Effective Octane And Efficiency Advantages Of Direct Injection Alcohol Engines+

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Abstract

Ethanol is receiving great interest as an alternative fuel. Methanol is another alcohol fuel that could serve as a replacement for gasoline. Although it is currently receiving much less attention, it has the potential to play an important role. Like ethanol, methanol also has the advantage of being a liquid fuel and it can be produced from gasification of a variety of feedstocks using well established thermal chemical technology. These feedstocks include coal, natural gas, biomass and various types of waste. This paper discusses the high effective octane number and efficiency advantages of methanol and ethanol when used in direct injection engines. Octane number represents the resistance of a spark ignition engine to knock (unwanted detonation which can damage the engine). The high intrinsic octane numbers of ethanol and methanol are well known. However, a much greater effective octane number can be effectively realized through the knock resistance provided by the high level of vaporization cooling that occurs when methanol or ethanol is directly injected into the engine cylinders. A computational model is used in this paper to determine the knock resistance and effective octane number of these alcohol fuels when they are directly injected. The model indicates that the effective octane numbers are around 160 for ethanol and 180 for methanol. The high compression ratio, high degree of turbocharging and aggressive engine downsizing enabled by the high effective octane number of methanol could provide an efficiency gain of 30 –35% (for combined city-highway driving) relative to conventional port fueled gasoline engines. An additional gain of around 10% can be obtained by using reforming of methanol to enable ultra lean operation at low loads. The combination of these gains could thus potentially provide an efficiency gain of 40–45% for direct injection methanol engines. This efficiency gain is significantly greater than the typical 25–30% gain of turbocharged diesel engines.

I. Introduction

Ethanol is receiving great interest as a transportation fuel, particularly in the United States. There is also renewed interest in methanol. Like ethanol, methanol has the advantage of being a liquid fuel and it can be made from a gasification of a variety of feedstocks using well established thermochemical technology. These feedstocks include coal and natural gas. Methanol can also be produced from a wide range of biomass including municipal waste, and also from industrial waste. It can thereby serve as low carbon emitting fuel. Methanol can thus be as an important option for replacement of gasoline.

There is considerable recent interest in China in methanol derived from coal. A program aimed at production of methanol powered demonstration fleets has been initiated by Cheri, a leading Chinese automobile manufacturer, and there are plans in China for certification of methanol-based fuels in early 2008 [Weigou]. In addition, there is interest in Sweden in biomass-derived methanol [Volvo]. Although there is little US interest in methanol at present [Ramadan, George] methanol was given significant consideration as an alternative transportation fuel in the 1970s and 1980s [Reed, Nichols]. Although there was some concern about the lower energy density/driving range and higher toxicity relative to gasoline, a considerable effort was made to explore the use of methanol in conventional port fuel injected cars. It included demonstration vehicles and fueling stations.

Progress in turbocharged, direct injection gasoline spark ignition engines opens up new possibilities for maximizing the benefits of using methanol. This paper investigates the effective octane number and efficiency advantages of direct injection engines that use methanol as a fuel. The effective octane number for ethanol is also computed and compared with that of methanol. Methanol and ethanol have important effective octane number advantages result from the large amount of evaporative cooling that results when they are directly injected into the engine cylinders. This evaporative cooling is very effective in suppressing knock (unwanted spontaneous detonation). The ability of the resistance of a fuel to knocking is given in terms of its octane number. Octane number is an important measure of performance and efficiency that can be obtained from a spark ignition engine.

Ethanol and methanol have a high intrinsic octane numbers. However, a much larger octane number is effectively obtained by the evaporative cooling that occurs when methanol is directly injected. The high level of knock resistance of directly injected methanol, which is represented by its high effective octane number, allows operation at much higher levels of engine power density and compression ratio. This makes it possible to use of small, highly turbocharged, high compression ratio engines to produce the same performance as much larger engines while providing a large increase in efficiency.

This examination of the capabilities for direct injection methanol engines draws upon the more extensive investigations of direct injection ethanol engines [Cohn, Bromberg] which can also benefit from a large increase in knock resistance provided by evaporative cooling. This paper builds on that work and determines the effective octane number for directly injected methanol. The effective octane number of methanol is significantly higher than that of ethanol due to its higher heat of vaporization, This higher effective octane number makes it possible for direct injection methanol engines to further improve on the benefits of direct injection ethanol engines.

In addition to its very high effective octane number, methanol has the advantage that it much easier to reform into hydrogen-rich gas than ethanol and other fuels. On board reforming of methanol could thus be attractive as means to enable ultralean engine operation at low loads by addition of reformer generated hydrogen-rich gas. Ultra lean operation at low loads can serve as means to further improve engine efficiency. The combination of higher efficiency from direct injection and from ultra lean operation can provide a substantial offset to the lower range of methanol power vehicles in comparison to gasoline powered vehicles (conventional methanol engine vehicles have approximately half of the range of gasoline powered vehicles for the size fuel tank due to the lower energy density of methanol).

II. Direct Injection Ethanol Engines

Interest in the use of ethanol is increasing in the United States and worldwide. Ethanol is currently used in the U.S., both as blending agent in gasoline (at a 10% level as an oxygenate which reduces carbon monoxide emissions) as well as a stand-alone fuel in the form of E85 (nominally 85% ethanol, 15% gasoline). US automakers have made flexible fuel production vehicle vehicles that can be operated on E85, gasoline or mixtures of these fuels. There is a major effort in the US to augment corn based ethanol production with ethanol produced from cellulosic material by biochemical processes. Gasification can also be used to produce ethanol from these materials along with methanol as a co-product. SAAB in Sweden has been promoting ethanol-gasoline blends in flex fuel vehicles, using a technology described as BioPower [See, for example, West]. Brazil has a large fleet of ethanol-powered vehicles, as well as a well established distribution system for ethanol derived from sugar. [Kremer].

We have investigated the use of the high knock resistance from evaporative cooling of directly injected ethanol. [Cohn, Bromberg]. The directly injected ethanol can be used as a stand-alone fuel in the form of E85. E85 can also be used as an on-demand octane additive for engines that are primarily fueled by gasoline. If an appropriate amount of ethanol from a second tank is directly injected into the cylinder of a spark-ignition gasoline engine at high load, the resulting prevention of knock allows for both increased compression ratio and increased turbocharging [Cohn]. The increased turbocharging allows substantial downsizing, *i.e.* replacing a large engine with a smaller engine that operates more efficiently while producing the same performance.

Initial modeling calculations indicate that knock-free operation with compression ratios of 12–14, together with boosting with a turbocharger in the range of 2.0–2.5 atmospheres, is possible with 100% DI (Direct Injection) ethanol operation [Bromberg]. This is a very large improvement relative to conventional port fuel injected engines which use 87 octane gasoline and operation with a compression ratio of 10 and a pressure of around 1 atmosphere (naturally aspirated).

An on-demand ethanol boosted gasoline engine operating with gasoline alone at low loads and DI ethanol addition from a separate tank to prevent knock at high loads, can provide a 25–30% improvement in fuel efficiency in typical city-highway driving, compared to a port-fuel injected spark-ignited naturally-aspirated engine [Cohn]. The required amount of ethanol use can be less than 5% of gasoline use.

Direct Injection engines using ethanol as either the primary fuel or as an octane boosting fuel could thus provide approximately the same efficiency gain as turbocharged diesels or typical hybrid gasoline-electric powertrains. The incremental cost for this efficiency gain is a fraction of the incremental cost for these two high efficiency options. This is due to the lack of the need for the expensive exhaust aftertreatment system and the very high pressure fuel injection system required for turbodiesel vehicles and the expense of the battery and electric propulsion system used the gasoline -electric hybrid.

III. Physical-chemical properties of methanol and ethanol

Table 1 shows the properties of gasoline, ethanol and methanol [SAEJ1297, Hunwartzen]. Ethanol is reported as having an octane rating of 129 (RON) and 102 (MON), with a combined octane rating of 115 ((R+M)/2). Methanol reported as having an octane rating of 133 (RON) and 105 (MON), with a combined octane rating of 119 ((R+M)/2). In contrast the combined octane rating of regular gasoline is 87 and that of premium gasoline is 93.

A simplified cooling effect has been estimated in Table 1. ΔT in Table 1 refers to the change in temperature of a stoichiometric mixture when the alcohol evaporates, assuming constant air properties. It is an indication of the evaporative cooling property of the fuel, as opposed to an absolute number, which depends on initial temperature, evaporation rate, time of injection, compression heating during evaporation, and other complications in the real system. In a stoichiometric mixture, ethanol has an evaporative cooling of about 4 times that of gasoline, while methanol has the effect of about 9 times larger than gasoline. These numbers are large, and projection of the effect of the evaporative cooling of ethanol on allowed turbocharging and compression ratio have been presented elsewhere [Bromberg].

Table 1. Properties of the alcohol fuels and gasoline

Fuel type		Gasoline	Ethanol	Methanol	Methanol with cosolvent 50% methanol /TBA
Chemical formula			CH3CH2OH	CH3OH	
RON			129	133	114
MON			102	105	96
(R+M)/2			115	119	105
Specific gravity	kg/l	0.75	0.794	0.796	0.789
Net heat of Combustion (LHV)	MJ/l	32	21	16	21
Net heat of Combustion (LHV)	MJ/kg	43	27	20	27
Latent heat of vaporization	BTU/gal	800	2600	3300	2500
Latent heat of vaporization	MJ/kg	0.30	0.91	1.16	0.88
Vaporization energy/heat of combustion		0.007	0.034	0.058	0.033
Stoic air/fuel ratio		14.6	9	6.4	8.8
Equiv. Latent heat of vaporization	MJ/kg air	0.02	0.10	0.18	0.10
ΔT air	K	-28	-138	-246	-137

IV Effective Octane model

The octane rating of a fuel is a measure of ability of the unburnt end gases to resist knock, that is, spontaneous ignition of the fuel, under the specified test conditions. Ideally, a fuel should resist ignition before arrival of the flame-front in the piston. The octane rating of the fuel is dependent on its composition.

There are specific engine conditions to determine the octane rating of a fuel. These tests are carried out in a CFR (Cooperative Fuels Research) engine. Two numbers have been used historically, the Research Octane Number (RON) and the Motoring Octane Number (MON). The conditions for the CFR engines used to determine octane of fuel are shown in Tables 1 for RON conditions and 2 for MON conditions.

Table 2. Engine conditions for Research Octane (RON)

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TIFF (LZW) decompressor
are needed to see this picture.

The conditions of the Motor Octane Number method represent severe, sustained high speed, high load driving. For most hydrocarbon fuels, including those with either lead or oxygenates, the Motor Octane Number will be lower than the Research Octane Number.

Table 3. Engine conditions for Motor Octane (MON)

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are needed to see this picture.

In this paper, the effective octane of the alcohols is determined using a computational model for the engine and the air/fuel chemistry. The knocking model is a modification of the model that has been described before [Bromberg]. The model uses pressures and temperatures from the literature on the characteristics of a Cooperative Fuels Research (CFR) engine, used to determine octane properties of the fuel. The Rate of Heat Release

(RHOR) has been adjusted until the peak pressures determined experimentally for a given fuel composition with a given octane number. The octane requirement of the engine is determined using Primary Reference Fuel (PRF) mixtures of isooctane (assigned an octane value 100) and n-heptane (assigned an octane value of 0) mixed by volume. The octane of a gasoline blend is determined by adjusting the CFR engine conditions operating with the gasoline blend until it knocks. With the same CFR conditions, the fuel is replaced with PRF mixture, and the composition of PRF fuel is varied until there is knock. The gasoline is then assigned the octane of the PRF mixture that knocks at the given engine conditions.

The pressure and temperature evolution in the cylinder CFR engine adjusted for 85 octane RON is shown in Figure 1. These are the CFR engine RON conditions (compression ratio, spark advance, inlet manifold pressure, air and water temperatures) for which Figure 2 shows the corresponding pressure and temperature for MON. The temperature and pressure data were kindly provided by Vikram Mittal [Mittal].

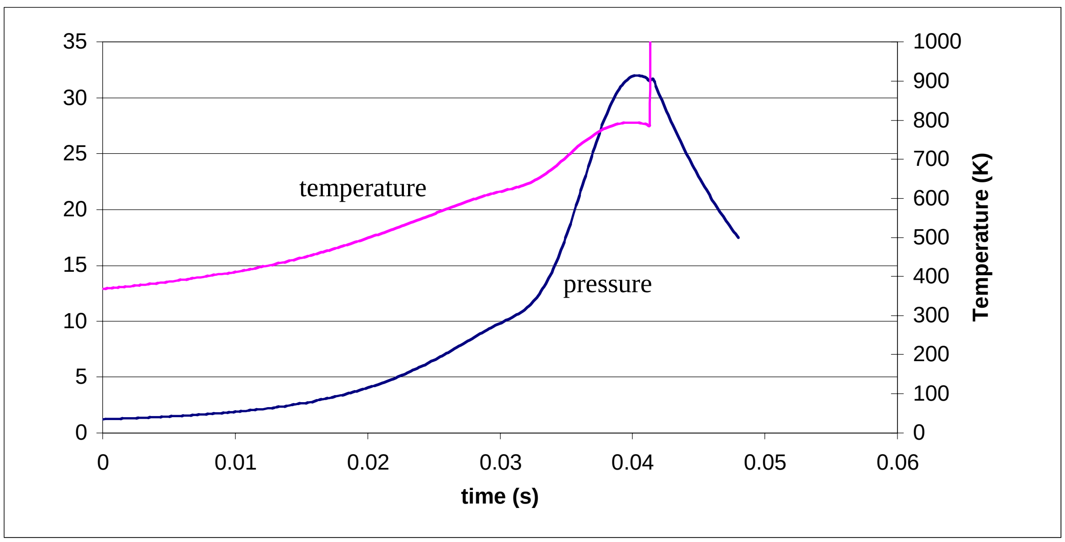

Figure 1. Pressure and temperature profiles for a CFR engine set for 85 RON fuel

Figures 1 and 2 the pressure and temperatures are shown as a function of time, not as a function of Crank Angle (CA), as is usually the case. The origin in Figures 1 and 2 refer an initial crank angle of ~120 CA before TDC (Top Dead Center).

The time of knocking is different for both conditions, as the engine speed is different from RON and MON.

The previous model [Bromberg] has been modified to determine the effect of direct alcohol injection on the octane of the port-fuel injected (PFI) fuel. The temperature of the air fuel mixture, at t=0 is decreased by the evaporation of the alcohol, which is assumed to evaporate instantaneously. The effects of finite fuel injection and evaporation time will be considered in the future, using a more complete description of the engine, including composition of the cylinder charge that includes the residuals (the exhaust gases left in the cylinder after the exhaust stroke).

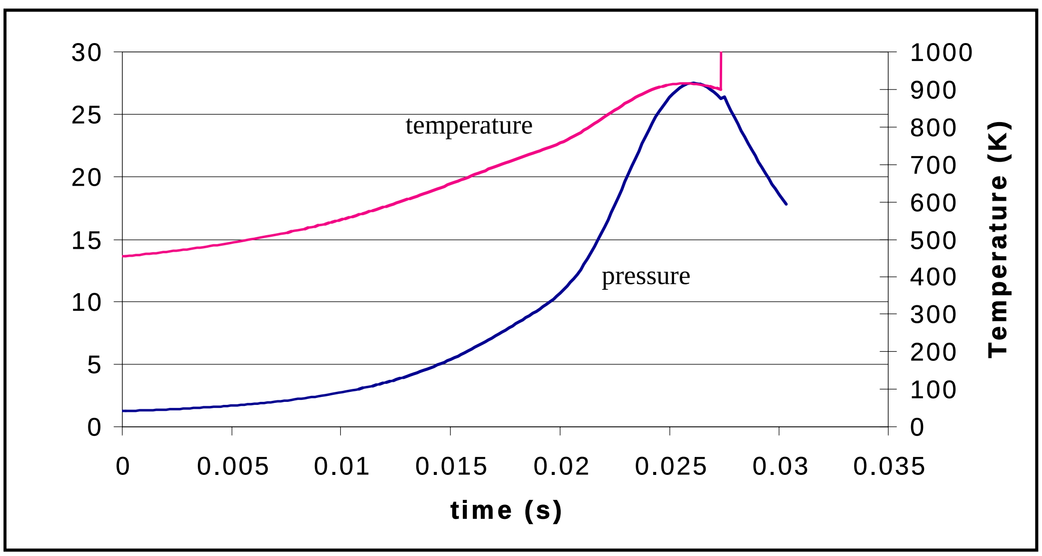

Figure 2. Temperature and pressure corresponding to CFR engine conditions of 85 MON.

The model assumes that the process is adiabatic, and the cylinder charge does not exchange energy with the cylinder walls. This assumption was investigated, and resulted in about a 20 K difference in the temperature profile, which is substantial. However, as the process means to provide relative knock conditions, it is expected not to have much of an influence on the results. The amount of PFI fuel is adjusted to compensate for the directly injected alcohol. The engine conditions are stoichiometric. The effect is more pronounced at the RON conditions, because of the slower engine speeds and thus longer times during which the cylinder charge can exchange energy with the walls.

The model follows the chemistry during the compression cycle, to the time where the fuel knocks in Figures 2 or 3.

For a given amount of DI alcohol, the model adjusts the octane of the port-fuel injected gasoline (modeled as PRF) until in knocking conditions are obtained. The value of the gasoline octane that results in knock for a given amount of DI alcohol is referred to as the degraded PRF octane. Then the effective DI octane of the alcohol is determined such that the overall octane of the fuel is 85, when averaged by volume (mixture fuel octane is the volume-average of the octane of the fuel components).

The process was performed for both RON and MON conditions for methanol and ethanol and various blends. The engine conditions are held constant, adjusted so that the octane requirement of the CFR engine corresponds to 85 octane fuel (for either MON or RON).

IV. Effective Octane Number Of Ethanol

Table IV shows the results for direct injection of ethanol. The calculations are performed for a given ethanol fraction addition, defined as the fraction of the fuel energy that is provided by the ethanol or a high concentration ethanol blend such as E85.   This fraction was 20%. For the present calculations, neat ethanol (E100) was used.

The computational model determines the gasoline octane number necessary to prevent knock when ethanol are directly injected into an engine that is port fueled with gasoline.

The first column in Table IV refers to the case when the engine conditions for RON 85 are run with PRF fuels exclusively. Although the knocking conditions for PRF should have been 85 octane, it was determined that instead the model predicts that the CFR engine knocks at an octane of 77.

Table IV. Ethanol effective DI octane and degraded PRF octane, for RON 85 engine conditions

	PRF octane	Degraded PRF octane	Ethanol use by volume	Ethanol DI effective octane
No ethanol	77			
10% E100		61	14%	175
20% E100		33	27%	195

The results from table IV (for RON) indicate that when ethanol is directly injected into the cylinder, with a fuel volume fraction of 14% (corresponding to 10% ethanol by energy), the octane of the port fuel injected gasoline can be reduced to 61 octane (i.e., 61% isooctane and 39% n-heptane, by volume), for comparable engine knocking conditions. The rules of mixtures (by volume) of the fuels can then be used to estimate the effective octane RON for the DI ethanol, and this is shown in the last column of Table IV. The deduced RON of DI ethanol is 185 +/- 10.

The case of MON is shown in table V. Similarly to the case of RON, the PRF that knocks for the engine conditions set for 85 MON is calculated in the model. In this case, the model predicts that for CFR engine conditions of 85 octane, the PRF fuel octane that resulted in knocking is 85, thus agreeing well with the experimental evaluation. Varying amounts of ethanol are directly injected into the cylinder, and the octane of the PRF is decreased until the model predicts knocking conditions. The effective MON of DI ethanol is calculated assuming mixture rules for the octane. The model estimates that the effective MON of DI ethanol is 150 +/- 5.

In the case of RON, the engine conditions for RON where fixed, assuming that the octane requirement of the engine is 77. As the process determines the knock by comparison, rather than direct calculations, it is expected that the octane determined in this manner is not a strong function of the original octane requirement of the engine.

Table V. Ethanol effective DI octane and degraded PRF octane, for MON 85 engine conditions

	PRF octane	Degraded PRF octane	Ethanol use by volume	Ethanol DI effective octane
No ethanol	85			
10% E100		74	14%	155
20% E100		64	27%	145
30% E100		48	39%	145

The reason for the discrepancy with the RON conditions between the knocking octane in the model and the experimentally determined knocking octane in the CFR engine is not clear. The discrepancy in the case of RON cannot be explained by neglect in the model of the residuals (the RON case is more throttled than MON and thus has a higher residual concentration). Neither can the difference be explained by neglect energy exchange with the walls. Both these effects would have the engine more resistant to knock, and thus would have further decreased the knocking octane of the fuel. The discrepancy provides some guidance as to the accuracy of the model.

According to the computational model the RON of the DI ethanol is around 180 while the MON is about 150. The combined (R+M/2) effective octane number is around 160. This number is substantially higher than the intrinsic octane rating of the ethanol (115) that does not take full advantage of the large heat of vaporization of the ethanol. It should be noted that direct injection of gasoline also increases the effective octane of the gasoline, but to a much lower degree than for ethanol or methanol.

To determine whether the effective DI octane of ethanol is dependent of the amount of the fuel that is injected, both RON and MON conditions where evaluated for varying amounts of ethanol DI. Tables IV and V show the calculated values of the degraded octane of port-fuel injected PRF fuel, for several fractions of directly injected ethanol, as well as the calculated values (using the octane mixture rule) of the effective octane value of ethanol. As shown in Tables IV and V, the calculated value of the effective DI MON of ethanol is approximately independent of the amount injected.

VI. Effective Octane Number Of Methanol

The same process was used to determine the effective DI octane of methanol. Because of the much large relatively heat of vaporization for methanol it was expected that the calculated octane would be substantially larger than those of ethanol.

Table VI. Degraded PRF octane and effective DI octane of methanol

		degraded PRF octane	Methanol additive effective octane	Methanol by volume
RON				
	No Methanol	77	--	
	methanol (5% by energy)	64	202	9.50%
	methanol (10% by energy)	45	221	18%
MON				
	No Methanol	85	--	
	methanol (5% by energy)	78	152	9.50%
	methanol (10% by energy)	67	166	18%

Table VI shows the results of the calculations. Indeed, the octane numbers are substantially higher than those of ethanol. In this case, the dependence on the effective DI octane of methanol is somewhat sensitive to the amount of methanol that is introduced. But the numbers are large even with this uncertainty. The combined octane number (R+M)/2 is around 180.

VII Direct injection Methanol Engines

A previously developed model [Bromberg] has been used to determine the minimum methanol addition that prevents knock in a direct injection engine. Basically a simple model is used to determine the conditions of the inlet manifold at the time of inlet valve shutoff. It includes the temperature increase due to turbocharging, intercooler, residuals, and charge cooling due to evaporation of the fuel. It has been assumed that the injection and evaporation is instantaneous, and occurs right at the moment of inlet valve closing. These conditions result in the largest decrease of the charge temperature, at constant-volume conditions (instead of constant pressure conditions) [Bromberg]. The effects of finite fuel injection and evaporation time will be considered in the future, using a more complete description of the engine, including composition of the cylinder charge that includes the residuals.

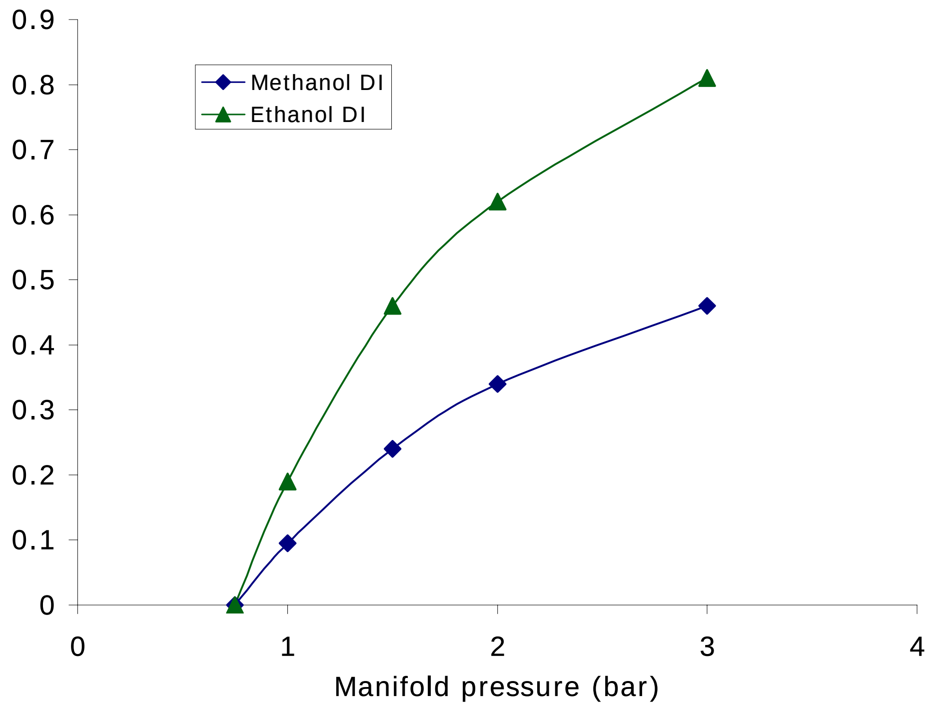

Figure 3. Alcohol fraction (by energy) required for borderline knock conditions, as a function of the manifold pressure, for a compression ratio of 10.

The results for low engine speed, 1000 rpm, are shown in Figure 3. The minimum alcohol requirement (in terms of energy fraction, the fraction of the total fuel power that is provided by the alcohol, the rest being provided by port-fuel injected gasoline, modeled as PRF with 87 octane) is shown as a function of the manifold pressure. The methanol requirements are compared with the required of ethanol (E100) reported previously [Bromberg].

Figure 3 indicates that DI methanol allows more than 30% increase in knock free turbocharging pressure at a given compression ratio, as compared with DI ethanol. In principle, this increased turbocharging allows for a downsizing by a factor of 3-3.5.

According to data analyzed by Shahed [Shahed] of number of comparable production vehicles, a factor of 10-30% downsizing results in an increased efficiency of 6-17% for diesel engines. A more conservative projection for increased efficiency is 4 -12 %. Assuming similar effects in a gasoline engine and that the downsizing trends extend to this very aggressive downsizing, the additional downsizing of ~ 30% could add a further efficiency gain of around 10% . It should be pointed out that appropriate turbochargers and reinforced engines would be needed to tolerate the higher in-cylinder pressures. The latter decreases the efficiency gain slightly, due to increased friction.

The further gain could result in an efficiency gain for a direct injection methanol engine of 30 to 35% relative to a port fuel injected gasoline engine. The methanol direct injection engine could be operated using methanol as the primary fuel (most likely mixed with some gasoline such as an M85 mixture) or an on-demand octane boost additive to gasoline operation.

An additional increase in efficiency of vehicles that use methanol as the primary fuel could be obtained by using an onboard reformer to efficiently convert methanol into hydrogen-rich gas which would be used to enable ultra lean operation at low loads [Wyszynski]. Ultra lean operation reduces pumping losses and provides a higher thermodynamic efficiency through a more favorable ratio of specific heats.

Stoichiometric operation would be used at high loads with emissions controlled by a three-way catalyst (additional development will be needed to prevent a decrease in effectiveness of the 3 way catalyst after a transition from ultra lean to stoichiometric operation).

Methanol is much easier to reform into than ethanol and other fuels. Use of thermal decomposition reforming could be particularly advantageous since it produces a relatively high concentration hydrogen-rich gas and can be carried out at a relatively low temperature, opening up the possibility of exhaust gas reforming. Thermal decomposition reforming using a plasmatron reformer [Bromberg1] or endothermic catalytic reforming using exhaust energy may be especially attractive. The fast startup provided by the plasmatron reformer could also be useful in providing hydrogen-rich gas to alleviate the cold start problems of a methanol fueled engine.

The combination of high compression ratio and downsizing provided by direct methanol injection together with reformer enabled ultra lean operation at light loads could provide an efficiency improvement of 40 to 45% relative to a conventional port fuel injected gasoline engine. This increase in efficiency is significantly greater than representative efficiency improvements of 25–30 % (combined city and highway driving) for turbocharged diesel engines with an advanced exhaust aftertreatment system (that includes NOx treatment and a particulate filter) and could be achieved at a lower cost. It is also greater than the typical 25–35% increase in efficiency that is obtained in gasoline-hybrid electric vehicles.

A 40–45% improvement in efficiency would also provide a significant offset to the range disadvantage of methanol fueled vehicles. With this improvement the range relative to a conventional gasoline engine with a similar size fuel tank would increase from approximately 50% to approximately 70%.

Conclusions

The effective direct injection octane numbers for ethanol and methanol have been estimated using a computational model. The combined effective octane number (RON +MON)/2 is around 160 for ethanol and 180 for methanol. The high effective octane number for methanol indicates the exceptional potential that methanol can have either as a primary fuel or as an octane boosting additive for enhanced performance and efficiency when gasoline is the primary fuel.

Direct injection of methanol could provide an efficiency gain which is equal to that of a gasoline-electric hybrid or turbodiesel at a much more affordable cost. Moreover when methanol is used as a primary fuel, reformer enabled ultra lean operation at low loads could provide a further efficiency gain of 10%.

These combined gains in a direct injection methanol engine could potentially provide an engine efficiency improvement of 40–45% relative to conventional port fueled gasoline engines. This efficiency improvement is greater than that of turbodiesels and gasoline-electric hybrids. The potential for a relatively low cost, high efficiency engine using directly injected methanol as a primary fuel provides additional motivation for consideration of methanol production from coal; natural gas; biomass including municipal waste ; and industrial waste as an alternative fuel to gasoline.

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