

Simulation of High Efficiency Heavy Duty SI Engines Using Direct Injection of Alcohol for Knock Avoidance

Paul N. Blumberg and Leslie Bromberg
Ethanol Boosting Systems LLC

Hyungsuk Kang and Chun Tai
Volvo Powertrain North America, Mack Truck, Inc.

Copyright © 2008 SAE International

ABSTRACT

The use of direct injection (DI) of a second fuel, ethanol or methanol (or their concentrated blends), is explored, via simulation, as a means of avoiding knock in turbocharged, high compression ratio spark-ignited engines that could replace diesels in certain vocational applications. The Ethanol Turbo Boost™ concept uses the second fuel only under conditions of high torque to avoid knock, while using only conventional gasoline throughout the rest of the engine operating range. This approach is an attractive alternative for heavy duty vehicles that operate intermittently at high torque and within a confined locale, reducing the logistical issues of supplying the knock-suppressing fuel.

The combination of GT-Power for engine calculations and a sophisticated chemical kinetics code for predicting knock were used in the study. After benchmarking the engine model against experimental data from an 11-liter heavy duty diesel engine, the 13-mode emissions speed/load points were investigated operating in ethanol boosted SI mode at a compression ratio of 14:1. For the baseline 11-liter case, two additional points were added: one with a higher, knock-free torque at the B-rpm (limited to 190 bar cylinder pressure); and one at 2100 rpm to achieve higher horsepower.

The ethanol boosting technology produces very high specific output, as the engine operates stoichiometrically (with three way catalyst for emission control) and can also operate at higher maximum engine speed. For a given engine size, it was determined that the ethanol-boosted SI engine could operate with about twice the torque and at higher horsepower than the baseline diesel engine. Consequently, a scaled, downsized 7-liter engine was simulated, which exhibited higher predicted efficiency than the baseline 11-liter diesel engine over most of the B-rpm torque range of the 13-mode test.

The paper evaluates E85 and methanol as the knock-suppressing fuels. Relative to E85, the use of methanol

reduces the storage requirements of the second fuel by about a factor of two. Further, the SI engine can operate with premium gasoline at the B50 point without any knock-suppressing fuel (e.g., if it is exhausted) with the use of DI gasoline and aggressive spark retard.

INTRODUCTION

The demand for high fuel efficiency is increasing due to environmental concerns, the desire to reduce petroleum use and increasing fuel costs. While diesel engines have traditionally been shown to be more efficient than conventional spark ignition engines, they must overcome substantial hurdles in order to comply with emission regulations.

On the other hand, emissions from gasoline engines have been reduced to very low levels through the use of the highly developed and effective three-way catalyst. The phenomenon of knock in spark ignition engines is a major factor that prevents it from reaching increased efficiencies. In general, the additional efficiencies that could be achieved if knocking phenomena could be prevented derive from increased compression ratio and engine downsizing with increased boost. Compared to heavy duty diesel engines, in particular, operation at stoichiometry at constant torque/power requires less turbocharging and overall engine mass flow. Furthermore, in achieving higher efficiency, it would be advantageous to use renewable fuels [1, 2, 3, 4, 5, 6].

A novel approach to avoid knock in spark ignition engines has been developed that exploits the use of direct injection of an alcohol in an otherwise conventionally fueled gasoline engine employing port fuel injection. In this paper, the concept is described and compared with a conventional heavy duty diesel engine as a baseline. The concept of direct alcohol injection for knock control is first presented. The computational model is then described. The results of simulation comparisons between a conventional diesel engine and three alcohol-enabled, high compression,

turbocharged, spark ignited engines are described: the first engine uses the same engine size as the diesel baseline with ethanol in the form of E85 as the direct injected fuel; the second, a downsized more highly turbocharged engine with E85 as the DI knock suppressing fuel; and the third, similar to the second, but with methanol as DI fuel.

ALCOHOL BOOSTED CONCEPT

The ethanol boost concept was originally developed at the Massachusetts Institute of Technology. The ethanol boost technology [7, 8, 9, 10] uses direct injection (DI) of a knock-suppressing second fuel when the engine is prone to knock (usually at conditions of high torque). The cooling, which derives from the high latent heat of vaporization of the knock-suppressing fuel, typically a lower alcohol such as ethanol or methanol, is primarily responsible for the knock suppression. Due to the charge cooling from the DI process, the effective octane rating [11] greatly exceeds the chemical octane rating that these fuels would exhibit using conventional induction methods such as port fuel injection (PFI). In the ethanol-boosted concept, DI of the knock-suppressing fuel is used only in the amount required to prevent knock and gasoline is supplied to the cylinder by conventional PFI. Since the engine operates at stoichiometry (using a typical O_2 feedback sensing system), a very high specific torque output can be produced while emissions can be maintained at low levels through the well-proven and relatively simple three-way catalyst system without the use of EGR as a major diluent. The technology opens the possibility of a spark-ignited gasoline engine operating at high compression ratio (12 – 14) and high boost ratios of 2.0 – 2.5 times ambient pressure, which is sufficient to produce a torque output equivalent to or greater than more highly turbocharged heavy duty diesel engines operating lean with significant EGR.

The ethanol-boosted technology offers an attractive alternative to diesel engines in light duty applications and in certain heavy duty vocational uses involving central refueling where the need for a second fuel would not pose a significant problem. It avoids the cost of a complex emission control system and the very high-pressure fuel injection system in favor of a gasoline type DI injection system (~130 – 150 bar) and three-way catalysts. Further, due to the high specific output at stoichiometry (compared to lean and EGR-diluted diesel operation at high torque needed to control NO_x emissions), an engine of smaller displacement can produce the required torque and power and be operated at a higher top speed, if desired. Under these conditions, the ethanol-boosted engine can be as efficient (as measured by BTE, brake thermal efficiency) as the replaced diesel and have lower specific CO_2 emissions as well. However, due to the lower energy density of gasoline and the second fuel compared to diesel fuel on a volumetric basis, the volumetric fuel

consumption will be higher, as measured in liters (or gallons) per hour.

The concept has been demonstrated and proven in systematic dynamometer tests at Ford, in collaboration with EBS [12]. In addition, Honda has independently investigated the concept [13].

The ethanol-boosted concept is being developed by Ethanol Boosting Systems LLC, a small spin-off company from MIT. The Volvo Powertrain (VPT) Division North America (VPT) of Mack Truck, Inc. and EBS undertook a short analytical study to examine the applicability of ethanol-boosted technology to the VPT MD11 diesel engine.

COMPUTATIONAL MODEL

A combined model to investigate the direct injection of alcohol in a spark ignition engine was constructed. The model consists of two modules. The first module models the engine flows, pressure and temperature evolution (including the effect of alcohol evaporation and heat losses), residuals, self-consistent turbocharger, etc. The second module performs the chemical kinetic evaluations using the pressure evolution and composition of the cylinder charge determined from the first model.

ENGINE MODEL - The engine model is built upon the GT-Power platform supplied by Gamma Technologies Inc. A single cylinder GT-Power, intercooled, turbocharged model, equipped with DI and PFI dual fueling capability was used for the calculations. It employs a two-zone combustion model so that temperatures in the unburned gas can be tracked separately. The model also has a built-in finite element cylinder temperature solver so that the effects of speed and load on heat transfer are included the gas temperature calculation.

Conventional valves and timing of the baseline MD11 [14] were used in the calculations (*i.e.*, there was no use of VVT or VCT at lighter loads). No EGR has been used in the calculations even at the light load points to reduce throttling losses. The compression ratio of the engine is assumed to be 14:1.

Peak cylinder pressure, air and EGR flow rates, temperatures and pressures upstream and downstream from the turbocharger, and information of pressure and temperature in the inlet manifold were used to calibrate the MD11 baseline engine operation (on diesel). The calibration was performed at the B100 point.

The dynamics of alcohol vaporization have substantial impact on the temperature of the unburned "end gas" in which knock occurs. It is assumed that the alcohol is completely vaporized by IVC. The effect of in-cylinder ethanol vaporization on unburned mixture temperature was calculated from the thermodynamic properties of the

alcohol, with imposed evaporation rates. The GT-Power model was modified to include a fuel with E85 properties, representing a concentrated form of ethanol, and contains its own template for methanol. The E85 was composed of 80% ethanol and 20% gasoline, which is in the typical range for an 85% *denatured* ethanol and gasoline mixture.

Ethanol has a high latent heat of vaporization, about three times that of gasoline, as shown in Table 1. The latent heat of vaporization is even larger for methanol. The ratio of heat of vaporization to the heat of combustion for either alcohol to that of gasoline is even higher, due to the lower heat of combustion of the alcohol relative to gasoline. The DI vaporization model allows specification of the half-life of the injected fuel in the liquid state prior to vaporization (assuming exponential evaporation). The half-life was chosen to ensure complete vaporization by IVC. In the present calculations, the port-fuel injected gasoline is 50% vaporized at the time of injection. Since the heat of vaporization of gasoline is low, this does not have a significant impact on the results. It is assumed that the alcohol is injected close to the boiling point, thus only the heat of vaporization results in charge cooling.

Combustion timing and duration have been investigated. It is assumed that the 10%-to-90% combustion duration (CA1090) of all the SI points is 25 CA degrees. This is achievable through the use of the right type of turbulence (*i.e.*, tumble) and possibly aided by dual ignition. As for combustion timing, MBT is assumed at all points that do not require alcohol injection. The peak BTE at MBT was determined, via analytical sweeps of the 50% burned point (CA50), to occur at a CA50 value of 7.5 CA degrees ATDC. When alcohol is required (because of knock), a 7.0 CA degree combustion retard was applied to CA50 in order to minimize the alcohol requirement. A small amount of combustion retard has a very pronounced effect on peak temperatures and pressures and a much smaller effect on thermal efficiency, while at the same time minimizing the consumption of the second fuel.

For the turbomachinery, a compressor efficiency of 80% has been assumed, with a turbine efficiency of 72%. Downstream from the compressor, an intercooler with an efficiency of 95% has been assumed.

Premium gasoline (98 RON) has been used as the primary fuel, introduced through PFI. Two DI knock-suppressing fuels have been considered: E85 (an available concentrated form of ethanol), and M100 for methanol.

CHEMICAL KINETIC MODEL FOR KNOCKING - The model developed by Bromberg [8] has been modified in order to determine the knocking tendency of an engine. In order to provide useful predictions of knock suppression throughout the engine operating regime, the end-gas conditions were modeled using a volumetric

compression of the unburned end-gas mixture. The method used in reference [8] to determine the pressure/temperature evolution of the end gas has been replaced with results from the engine model described in the previous section. Initial temperature for the calculations, as well as the pressure profile (both from GT-Power), were used as inputs to the chemical kinetics code. The chemistry model was adiabatic, but the GT-Power included heat exchange with the cylinder walls (as described in the previous section). As the chemistry in the end-gas mixture was not included in the overall cylinder pressure, the model breaks down at incipience of knock, but is adequate to determine knock occurrence. The addition of the directly injected alcohol, cools down the air-fuel mixture and affects the air-fuel chemistry.

The chemical kinetics code CHEMKIN 4.1 [15] 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.* [16] to represent the auto-ignition of the fuel. The mechanism also includes ethanol and methanol chemical models [17].

Table 1. Physical properties of gasoline, ethanol and methanol; from reference [18]

Fuel type		Gasoline	Ethanol E100	Methanol M100
RON			129	133
MON			102	105
(R+M)/2			115	119
Specific gravity	kg/l	0.75	0.794	0.796
Net heat of Combustion (LHV)	MJ/l	32	21	16
Net heat of Combustion (LHV)	MJ/kg	43	27	20
Latent heat of vaporization	BTU/gal	800	2600	3300
Latent heat of vaporization	MJ/kg	0.30	0.91	1.16
Vaporization energy/heat of combustion		0.007	0.034	0.058
Stoic air/fuel ratio		14.6	9	6.4
Equiv. Latent heat of vaporization	MJ/kg air	0.02	0.10	0.18

The gasoline is modeled as a mixture of primary reference fuels. RON 98 octane (premium gasoline) was used (2% n-heptane and the balance isooctane, by volume). E85 properties were constructed by using 80% ethanol and 20% gasoline by volume, respectively.

The amount of alcohol (and the resulting initial temperature) is varied in the engine module and the chemical kinetics module is then used to determine whether the specified conditions result in knocking. The knock chemistry is stiff; and small initial temperature changes result in substantial changes in the timing of the auto-ignition. At the B100 condition, auto-ignition onset varies by 1 crank angle degree for one degree of change of the initial temperature (corresponding to 1% change in ethanol energy fraction). Thus the alcohol required to avoid knock is not very sensitive to the timing of auto-ignition.