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INFLUENCE OF WATER CONTENT IN ETHANOL-WATER BLENDS ON THE PERFORMANCE AND EMISSIONS OF AN SI ENGINE

¹Sileghem, Louis^{*}; ¹Casier, Ben; ¹Coppens, Alexander; ¹Vancoillie, Jeroen; ¹Verhelst, Sebastian;

¹ Department of Flow, Heat and Combustion Mechanics, Ghent University, Belgium

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ABSTRACT -

Ethanol is the most common alternative for conventional gasoline replacement in sparkignition engines. It holds multiple advantages over other renewable transportation technologies including energy density, distribution infrastructure compatibility and the possibility of efficiency improvement and pollutant emissions reduction. Most of the fuel grade ethanol is dehydrated to a minimum purity of 99,6 % before blending or direct use as fuel. As this process is the main energy consumer of the fuel production, it is clear that a large cost reduction can be realized by dropping or decreasing this energy demand. It was investigated if hydrous ethanol is an interesting fuel for flex fuel vehicles where driving range is not of primary importance. Performance and engine-out emissions of mixtures with 5% v/v, 10% v/v and 20% v/v water were compared to pure ethanol and gasoline on a 4 cylinder 1.8 1 PFI production engine.

TECHNICAL PAPER -

INTRODUCTION

Fossil fuels have been consumed in large quantities since the industrial revolution. The past decades, awareness has grown that we cannot solely depend on these fuels as energy carriers for transport applications. Oil reserves, climate change and air quality are factors that encourage to look at renewable alternatives. Constantly increasing world population and accompanying energy demand puts this challenge in an even bigger perspective. As electric and hydrogen powered vehicles and fuel cell technology are not ready for a full scale breakthrough, light alcohols like methanol and ethanol are presented as most promising fossil fuel replacement [1]. These liquid fuels are compatible with existing infrastructure and are usable as blend-in fuels for production cars in limited concentrations. Corrosion problems require correct material selection in flex fuel vehicles to enable durable engine operation on higher alcohol concentrations.

After a first emergence during the 70's and 80's in countries like Brazil and the United States, the interest in alternative fuels disappeared due to decreasing oil price and diminishing government support. As gasoline price is currently rising and this trend is expected to continue, liquid alcohols have again come to the attention as suitable substitutes. The lion's share of this fuel shift is commonly contributed by ethanol. This alcohol is produced by fermentation of sugars from any biomass containing sugar or starch (sugar cane, corn, beets,...). Efforts are undertaken to avoid interference with the food chain through research and development of next-generation cellulosic ethanol. After fermentation a 10 % ethanol-in-water solution is obtained, this water content is removed primarily by distillation as described in the next paragraph.

HYROUS ETHANOL

Economic aspects of ethanol production

The removal of most of the water content in fuel grade bio-ethanol has traditionally been considered as essential. Conventional distillation is used for the first part of the dehydration process. As water and ethanol form an azeotropic mixture at 95.63 wt% ethanol/4.37 wt% water, the last water content is removed through an energy intensive dehydration process. This is done by performing azeotropic distillation (involving additives like benzene, cyclohexane or toluene) or extractive distillation (adding a solvent to break the azeotrope). Figure 1 shows distillation energy as function of volumetric ethanol fraction. An exponential increase is observed at a concentration of 80 vol% ethanol [2].

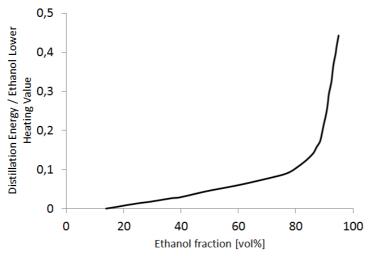


Figure 1 – Distillation energy required as function if purity [2].

These energy requirements determine a significant part of the total ethanol production cost. Distillation efficiencies are still improving thanks to optimization of process and installation, e.g. distillation step integration and more efficient heat utilization [3-5]. Another important efficiency gain is feasible through material development whereas molecular zeolite sieves present a valuable and energy efficient alternative when used in Pressure Swing Adsorption [6-8]. Nevertheless, it is clear that using hydrous ethanol directly as fuel (or as blending component with gasoline [9]) would imply a substantial economic advantage over fully denatured ethanol.

Mack et al. [10] reported that direct utilization of 35% ethanol in-water mixture reduces water separation cost to only 3% of the energy of ethanol and co-products (versus 37% for producing pure ethanol), and improves the net energy gain from 21% to 55% of the energy of ethanol and co-products. Although this mixture is not exploitable in existing production SI engines due to ignition limitations, numerical simulations of a HCCI engine predict the possibility of operation on this blend [2]. Mack et al. [10] tested this statement experimentally and reported a stable HCCI operation up to 40 wt% water.

Brazil has been a frontrunner regarding alcohol usage as fossil fuel alternative in production vehicles driven by extensive government support. Depending on ethanol supply, minimum mandatory blending percentages of 18 to 25 % ethanol in gasoline are instructed. Higher alcohol content blends are also marketed (e.g. the well-known E85) as is the hydrous ethanol presented as E100. This blend that can contain up to 7,4 % water content, is sold as standalone fuel.

Hydrous ethanol as fuel for internal combustion engines

It is well known that the light alcohols like ethanol have the potential to improve engine performance and efficiency thanks to some interesting properties. The most promising are [11]:

- High heat of vaporization, which in combination with the low stoichiometric air to fuel ratio leads to high degrees of intake charge cooling as the injected fuel evaporates.
- Elevated knock resistance, which is partly due to the considerable cooling effect. This opens opportunities for increased power and efficiency by applying higher compression ratios, optimal spark timing and aggressive downsizing.
- High flame speed which increases the tolerance for dilution, thus enabling qualitative load control using mixture richness or varying amounts of EGR.

In the appendix , the properties of gasoline and ethanol relevant to their use in internal combustion engines are summarized.

Adding water has an influence on the cooling effect. Water has a higher latent heat of vaporization and a higher specific heat capacity than ethanol. Because the stoichiometric air quantity (Ls) decreases with higher water content, the latent heat of vaporization per kg air increases significantly and this leads to an even bigger cooling effect of the intake charge. Adding water also results in an elevated knock resistance, due to the cooling effect and the water vapor dilution which both contribute to lower in-cylinder temperatures. The water vapor dilution of the air-fuel mixture yields a lower laminar burning velocity and lower adiabatic flame temperature. Because of the lower laminar burning velocity, the combustion process takes more time to complete and is less isochoric. The theoretical efficiency of the ideal Otto cycle forms the upper limit of the brake thermal efficiency and a less isochoric combustion yields a lower efficiency. Further, the longer combustion duration is reflected in a more advanced ignition timing. A lower adiabatic flame temperature and the lower in-cylinder temperature secure heat losses contributing to a higher efficiency.

Adding water to the ethanol also has some consequences concerning emissions. The formation of NO_x is strongly related to the in-cylinder peak temperature, the residence time in the cylinder and the presence of oxygen. All measurements in this paper are done at lambda equal to 1 thus there is no difference for the last factor. With the addition of water, there are two counteracting effects that can be expected. The slower combustion process and associated with this the more advanced ignition timing, could lead to increasing NO_x -emissions due to the longer residence time of the burned gases at high combustion temperatures. On the other hand the cooling effect of the ethanol-water blends combined with the lower adiabatic flame temperature is expected to lead to a decrease in the emissions. Normally the temperature dependency is the more dominant factor, so a decrease in NO_x -emissions can be expected with higher water content in the blend.

Because of the water dilution, the combustion process is expected to be less complete and the flame is expected to be more susceptible to flame extinction. Moreover, condensing water vapor can enlarge the quench layer. From this it can be expected that unburned fuel emissions and CO emission will increase.

EXPERIMENTAL SETUP

The engine tests were conducted on a 1.81 SI PFI 4-cylinder production engine modified to run on hydrogen, alcohol and gasoline. Table 1 shows the specifications. The engine is equipped with 4 alcohol compatible liquid fuel injectors (Racetronic 48INJL) which are fed through a stainless steel fuel rail.

| Cylinders | 4 inline | | |
|---|-------------------------|--|--|
| Valves | 16 | | |
| Valvetrain | DOHC with CVVT | | |
| Bore | 83 mm | | |
| Stroke | 82.4 mm | | |
| Displacement | 1783 cc | | |
| Compression Ratio | 10.3:1 | | |
| Injection | PFI | | |
| Max. revs | 6000 rpm (continuously) | | |
| ECU | MoTeC M800 | | |
| Table 1 Specifications of the test engine | | | |

Table 1 – Specifications of the test engine

A MoTeC M800 engine control unit is used to control ignition timing, start of injection, injection duration and intake valve timing. Cylinder pressure measurements were possible using a spark plug pressure sensor, a piezo-electric Kistler type 6118AFD13. A piezo-resistive Kistler type 4075A10 sensor placed in the intake manifold close to the inlet valves was used for pegging the cylinder pressure. The crank angle was recorded using a Kistler crank angle encoder type COM2611.

The exhaust gas components O2, CO, CO2, NO, NO_x were measured (O2: Maihak Oxor-P S710, paramagnetic; CO, CO2, NO, NO2: Maihak Multor 610, non-dispersive infra-red). For ethanol and gasoline a gravimetric fuel measurement was used. A direct reading of the air to fuel equivalence ratio λ is given by a Bosch wide band sensor and digital air/fuel ratio meter with calibrations for ethanol and gasoline.

Procedure

The results presented in this study were obtained during steady state operating conditions at various engine speeds and loads. The load was always controlled with the throttle valve. Load control using varying amounts of residual gas could not be considered since the engine does not have an external EGR system. The basic engine map, which prescribes injection quantity and ignition timing for ethanol, was adjusted for the ethanol-water blends through fuel trims and ignition advancement in order to keep lambda equal to 1 and maintain MBT (Minimum spark advance for best torque) timing. Stoichiometric operation was chosen in order to maximize the conversion rate of the commonly used TWC. Table 2 shows all tested operating points.

| λ | Torque | BMEP | Speed |
|-----|--------|-------|------------------|
| [-] | [Nm] | [bar] | [rpm] |
| 1 | 40 | 2.819 | 1500, 2500, 3500 |
| 1 | 80 | 5.638 | 1500, 2500, 3500 |

 Table 2 – Tested operating points

RESULTS AND DISCUSSION

The engine was fuelled with pure ethanol and three different ethanol-water blends (5% v/v, 10% v/v and 20% v/v water). The first blend is chosen at 5% v/v so the energy intensive

dehydration process could be excluded. The third blend is chosen at 20% v/v because in Figure 1, the exponential increase in distillation energy begins here. The second blend is chosen in between the two other blends to be able to optimally observe the evolution with increasing water content in the blends. In this paper, v/v% is always the volume percentage before mixing. The final volume differs from the sum of the beginning volumes of the 2 components (ethanol and water) due to differences in the way liquids having different molecular sizes 'pack' together.

Performance

In Figure 2, the brake thermal efficiency of the ethanol-water blends is shown at a load of 40 Nm and various engine speeds. This load is suited for a light acceleration or cruising in a high gear at low rpm. There are no significant differences between all ethanol-water blends, which is remarkable for a blend with 10% v/v (26.44 mole%) and even 20% v/v (44.72 mole%) of water. If we compare this with gasoline (Euro 95), we see a 1-2% pt improvement for the ethanol blends.

This improved efficiency was expected as ethanol has a higher burning velocity so the combustion occurs more isochoric. A second positive influence is the high latent heat of vaporization and high heat capacity of ethanol which result in lower in-cylinder temperatures and associated smaller cooling losses.

Despite the fact that all differences between the ethanol-water blends fall within the experimental uncertainty, it is still possible to observe a certain trend with the addition of water. At lower speeds pure ethanol seems to have a higher efficiency than the other blends, while at higher rpm the ethanol-water blends seems to have higher efficiency than the pure ethanol. A possible reason for this trend is that the lower laminar burning velocity of ethanol-water blends has less influence on the actual burning velocity at higher engine speeds because of the higher flow turbulence at high speeds. The same trend was observed for methanol-water blends [12].

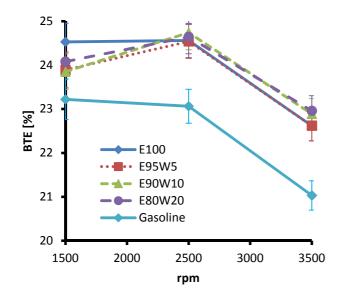


Figure 2 - Brake thermal efficiency at 40 Nm

The same results and trends were also found for the higher load of 80 Nm (see Figure 3). As the load increases, the efficiencies increase too and are a significant 5-7% pt higher than at the

40 Nm part load. The dominating effect for this improvement is the increase in mechanical efficiency with increasing load.

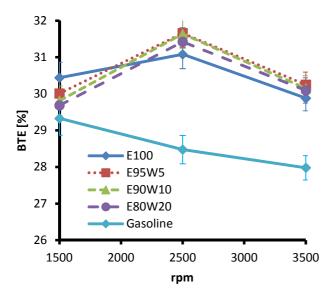


Figure 3 - Brake thermal efficiency at 80 Nm

With increasing speeds we see that the efficiency decreases slightly. There are various effects that play a role resulting in a decrease of the efficiency:

- The air (and fuel) flow increases to maintain the same load at higher engine speeds, so the flow losses are higher.
- In order to obtain this higher air flow, the throttle position will be more opened (Figure 4), consequently leading to lower throttle losses.
- The mechanical efficiency decreases with increasing rpm, through the higher friction losses at these high speeds.
- The last effect is the decreasing relative heat losses with increasing engine speed, so the absolute heat losses increase less than linearly with increasing rpm.

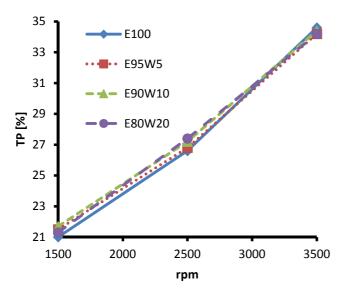


Figure 4 - Throttle position at 80 Nm

The addition of water to the ethanol decreases the LHV (Lower Heating Value) of the blend. This means more fuel will have to be injected to maintain the same load with the ethanolwater blends, which results in a significant increase of the BSFC (Figure 5). For the same fuel tank, the driving range will be shorter with increasing water content. This effect will be slightly counteracted by the rearrangement of the water and ethanol molecules, so that the blend will occupy less volume than the sum of volumes of the 2 components.

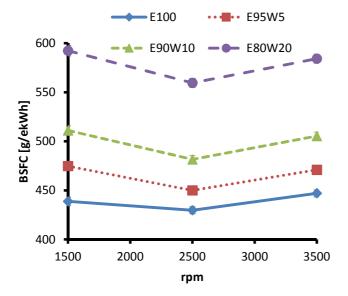


Figure 5 - Brake Specific Fuel Consumption at 80 Nm

In Figure 6, the volumetric efficiency is shown at the higher load of 80 Nm. The volumetric efficiency is defined as:

$$\eta_{v} = \frac{m_{fuel+air}}{\dot{m}_{theoretically}}$$

with $\dot{m}_{fuel+air}$ the actual mass flow of fuel and air entering the cylinders during the intake stroke and $\dot{m}_{theoretically}$ the theoretical mass flow that could enter the cylinders under reference conditions (= atmospheric conditions).

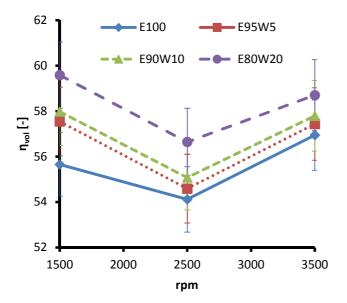


Figure 6 - Volumetric efficiency at 80 Nm

In Figure 4, the throttle position for the different fuels is shown and as can be seen, there is no big difference between the throttle positions of the different fuels. As a result, the difference in the volumetric efficiency is mainly caused by the cooling effect of the different methanol-water blends. From Figure 6, it is clear that the higher heat of vaporization of the water-methanol blends has a bigger cooling effect on the intake charge resulting in a higher volumetric efficiency.

Emissions

This section discusses the trends of NOx- and CO-emissions for the various ethanol-water blends. Emissions of unburned fuel were not measured because for flame ionization detectors as used in our exhaust gas analyzers, the reaction time for oxygenous hydrocarbons is impracticable long and thus realistic values are not possible. Oxygenated species such as unburned ethanol and acetaldehyde are commonly found in the exhaust gases of ethanol engines [13]. Using a flame ionization detector might thus lead to an underestimation of the total unburned hydrocarbons on ethanol operation.

Figure 7 shows the engine-out NOx-emissions for the various ethanol-water blends at the load of 80 Nm. The lower adiabatic flame temperature and cooler in-cylinder temperature due to the larger cooling effect and the water dilution explain the lower NOx-emissions on ethanol-water blends compared to on pure ethanol. This explains also the lower exhaust temperatures in Figure 8. The lower NOx-emissions at low rpm might be caused by elevated levels of internal EGR at these engine speeds. At this load, the vacuum in the intake due to throttling is quite considerable, so internal EGR levels can be expected to be important.

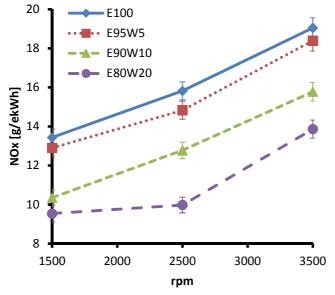


Figure 7 - NOx-emissions at 80 Nm

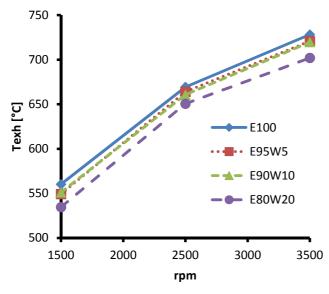


Figure 8 - Exhaust temperature at 80 Nm

In Figure 9 we see the CO-emissions of the various ethanol-water blends at the load of 40 Nm. As expected the emissions of the water containing blends are slightly higher than with the pure ethanol, because of the less complete combustion. This is also confirmed for the higher 80 Nm load. Nevertheless, all differences fall within the experimental uncertainties so it is not possible to be certain of this trend. In fact, a small deviation from the stoichiometric condition could have a bigger influence than the water content of the blends. A decrease in CO-emissions with increasing engine speeds is also observed, which potentially can be explained by the higher turbulence at these speeds which may result in a better combustion.

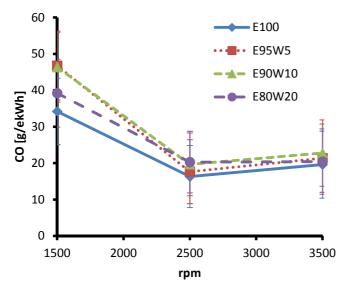


Figure 9 - CO-emissions at 40 Nm

CONCLUSION

Ethanol-water blends with 5% v/v, 10% v/v and 20% v/v were compared to pure ethanol and gasoline on a 4 cylinder 1.8 l port fuel injected production engine. Brake thermal efficiency is unaffected or even improved and remains higher than the efficiency for gasoline. The same

applies for pollutant emissions, NO_x emissions are significantly reduced with increasing water content due to lower in-cylinder temperatures. Even though driving range decreases significantly with increasing water content, significant production cost reduction may be decisive in consumer and manufacturer behavior. The trade-off between BTE, driving range and economic advantage gives reason to assume that an optimal water concentration would be situated in the 5-10 vol% range, which is conveniently close to the result from normal distillation and covers the `E100' blend currently used in the Brazilian market.

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APPENDIX

| Property | Gasoline | Ethanol | | |
|---|-----------|----------------------------------|--|--|
| Chemical formula | Various | C ₂ H ₅ OH | | |
| Oxygen Content by mass (%) | 0 | 34,73 | | |
| Density at NTP (kg/l) | 0,74 | 0,79 | | |
| Lower heating value (MJ/kg) | 42,90 | 26,95 | | |
| Volumetric Energy Content (MJ/I) | 31,70 | 21,29 | | |
| Stoichiometric AFR (kg/kg) | 14,4 | 9,0 | | |
| Energy per unit mass of air (MJ/kg) | 2,98 | 2,99 | | |
| Research Octane Number (RON) | 95 | 109 | | |
| Motor Octane Number (MON) | 85 | 98 | | |
| Sensitivity (RON-MON) | 10 | 11 | | |
| Boiling point at 1 bar (°C) | 25-215 | 79 | | |
| Heat of vaporization (kJ/kg) | ~305 | 838 | | |
| Reid vapour pressure (psi) | 7,00 | 2,30 | | |
| Mole ratio of products to reactants ^a | 0,937 | 1,065 | | |
| Flammability limits in air (λ) | 0,26-1,60 | 0,28-1,91 | | |
| Laminar burning velocity at NTP, | 33,0 | 38,5 | | |
| $\lambda = 1 \text{ (cm/s)}$ | | | | |
| Adiabatic flame temperature (°C) | 2002 | 1920 | | |
| Specific CO ₂ emissions (g/MJ) | 73,95 | 70,99 | | |
| ^a Includes atmospheric nitrogen. NTP: normal temperature | | | | |
| (293K) and pressure (101325 Pa) | | | | |