

Analysis of the Effect of Bio-Fuels on the Combustion in a Downsized DI SI Engine

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ABSTRACT

In this study the fuel influence of several bio-fuel candidates on homogeneous engine combustion systems with direct injection is investigated. The results reveal Ethanol and 2-Butanol as the two most knock resistant fuels. Hence these two fuels enable the highest efficiency improvements versus RON95 fuel ranging from 3.6 % - 12.7 % for Ethanol as a result of a compression ratio increase of 5 units. Tetrahydro-2-methylfuran has a worse knock resistance and a decreased thermal efficiency due to the required reduction in compression ratio by 1.5 units. The enleanment capability is similar among all fuels thus they pose no improvements for homogeneous lean burn combustion systems despite a significant reduction in NO_x emissions for the alcohol fuels as a consequence of lower combustion temperatures. In general, 1-Butanol and 2-Butanol emit higher amounts of HC emissions in all operation points combined with significantly increased particle emissions at high loads indicating a worse mixture formation. Alcohol fuels lead under cold conditions to a higher oil dilution which is significantly depending on the boiling temperature of the fuel. Hence, the usage of 1-Butanol as a pure fuel is critical.

INTRODUCTION

One major challenge for today's society is the sustainable satisfaction of its energy demand. Today, the entire transportation sector primarily uses fossil fuels. Despite the recent improvements of electrical vehicles, a total independence of internal combustion engines cannot be foreseen for the upcoming years.

Hence, the vision of mobility becoming free of greenhouse gas emissions can only be realized by a complete substitution of conventional fuels with bio-fuels. Politics promote this change by establishing constantly increasing quotes for bio-fuel blending to conventional fuel. The European Union for examples has specified the share of bio-fuel to be at least 10 % on an energetic basis by 2020.

In a short and mid term perspective this quote will most likely be realized using Ethanol as the blending agent for gasoline fuel. The availability of other bio-fuels, suitable for gasoline engines, from large scale production processes cannot be foreseen for the coming years.

Former work of the authors has revealed the potential and the challenges of increasing Ethanol blending with a special focus on direct injection engines. Using the same compression ratio, efficiency improvements can be gained as a result of an advanced more ideal combustion phasing at high loads due to improved knock resistance and reduced enrichment demand for component protection especially for charged engines. This leads to efficiency gains of E85 of up to 16 % at low engine speeds where differences are not caused by different levels of enrichment and 38 % at higher engine speeds /1/. These findings are in agreement with the results of several other researches /2/, /3/, /4/. Investigations with increased compression ratio have shown part load benefits of 0.6 - 1.6 %-points when raising the compression ratio by 1.5 units to 13 for pure Ethanol in /5/ while /6/ found a 7.4 % improvement in CO₂ emissions for Ethanol compared to RON95 fuel as a consequence of a compression ratio increase of 3 units to 12.5. However, the compression ratio adaptations are not performed on the basis of objective criteria, such as combustion stability or full load combustion phasing. This approach has been followed in another study of the authors in order to investigate the potential of mid-term Ethanol blending ratios of 20 % for CO₂ emission reduction via compression ratio adaptations to the higher knock resistance of the fuels. This has lead to a compression ratio increase of 2.2 units for an E20 blend with a research octane number (RON) of 102 enabling a CO₂ emission reduction of 3.3 % in the New European Driving Cycle /7/. The impact of Ethanol on homogeneous lean burn combustion systems using external mixture formation is reported for instance in /8/ and /9/ while impacts on stratified engine operation are studied in /10/. The high enthalpy of vaporization of Ethanol is especially

critical for cold starts. Investigations using in-cylinder gas sampling have shown that the Ethanol content diminishes with decreasing temperature and only the low volatile fuel fractions are evaporated, thus explaining the significantly higher enrichment demand for E85 compared to conventional fuels /11/. The high enrichment is also reported to lead to high oil dilution /12/. For direct injection engines, limitations can arise from pump capacity, however, multiple injection strategies can reduce wall film formation and thus improve evaporation and startability /7/, /10/, /13/. Since 2009, the only direct injection mass production engine capable of Ethanol contents up to E85 is the Audi 2.0l TFSI /14/.

Less information has been published on 1-Butanol, mostly, however, not exclusively, focusing on the near-term perspective of 1-Butanol blending to gasoline fuel. For this purpose, 1-Butanol has the advantage, that the required injection durations to achieve a stoichiometric air excess ratio are much closer to Gasoline than for Ethanol. Assuming a typical lambda control window of 25 %, pure 1-Butanol could be used in principle. This assumption of course falls short of the fact that the lambda control window is also used to compensate tolerances between engines and that a different start and warm-up calibration will be required for 1-Butanol due to the high enthalpy of vaporization. The existing literature concludes that 1-Butanol is a feasible fuel for gasoline engines and that efficiency and emissions are not adversely affected at least when compared to similar RON fuels /15/, /16/, /17/, /18/.

In a long term perspective a bio-fuel needs to be feasible for a combustion engine as a pure fuel and not only as a blending agent to conventional fuel. This might of course require certain adaptations of the engine hardware to the requirements of the new fuels as well as adapted engine calibrations. Besides feasibility for large scale and economic production the well-to-wheel balance needs to be in favor of every fuel that intends to alter the pathway towards Ethanol that is currently pursued. Consequently, the development of new synthetic fuels from bio-mass requires detailed knowledge of the entire process chain from preparation and conversion of biomass, the synthetic pathways up to the fuel-specific performance of an internal combustion engine. The Cluster of Excellence "Tailor-Made Fuels from Biomass" has adopted an interdisciplinary approach to determine the optimal bio-fuel components and their production processes as the long-term goal. The vision is to tailor the combination of fuel properties and combustion system to enable a high efficient homogeneous lean combustion at high loads and controlled auto ignition at low loads.

FUELS

Following this goal, each fuel was tested as a pure substance with purity grades > 95 %, in most cases even > 99 %. Besides the Butanol isomers, fuel molecules with a ring structure consisting of four carbon atoms and one oxygen atom combined with further functional groups seem promising candidates

with advantages in the well-to-tank balance. As a first fuel of this group, Tetrahydro-2-methylfuran was tested in comparison to 1-Butanol and 2-Butanol while Ethanol, Isooctane and conventional RON95 fuel serve as the state of the art bio- and non-bio-fuels to assess the findings with the other fuels. Table 1 summarizes the most relevant fuel properties with data taken from /19/, /20/, /21/, /22/, /23/, /24/, /25/ and /26/. Cross-comparing the table entries, some remarkable differences can be noted. Ethanol has the highest oxygen content of all tested fuels and consequently the lowest heating value. Comparing Ethanol and Isooctane, the enthalpy of vaporization differs by a factor of 3. The different stoichiometric air requirement intensifies this effect. The heat dissipated for a given identical cylinder charge at stoichiometric air excess ratio varies by a factor of nearly 5. Tetrahydro-2-methylfuran has the highest density and, together with Ethanol, the lowest boiling temperature among the pure substances.

Table 1: Fuel properties

	RON95	Isooctane	Ethanol	1-Butanol	2-Butanol	Tetrahydro-2-methylfuran
Carbon content / w.-%	84.47	84.12	52.14	64.82	64.82	69.72
Hydrogen content / w.-%	13.27	15.88	13.13	13.60	13.60	11.70
Oxygen content / w.-%	2.26	0.00	34.73	21.58	21.58	18.58
Density / kg/m ³	737	690	786	806	803	849
Viscosity / mPas	-	0.48	1.08	2.53	3.00	0.48
Surface tension / mN/m	-	18.35	22.10	24.37	23.11	24.56
Boiling temperature / °C	41.5 - 173.5	99	78	118	99	79
Enthalpy of vaporization / kJ/kg	~ 397	309	912	688	672	357
Stoichiometric air requirement / -	14.14	15.09	8.98	11.16	11.16	11.21
Lower heating value / MJ/kg	42.13	44.34	26.84	33.12	32.92	34.00
Mixture heating value (DI, $\lambda = 1$) / kJ/m ³	3446	3478	3538	3512	3491	3591
Research octane number / -	96.3	100	108.6	94	not det.	86

1-Butanol has the highest boiling temperature of the pure substances and, together with 2-Butanol, features the highest viscosity. The viscosity of 2-Butanol is more than 6 times higher than the lowest viscous liquid Isooctane which will influence the friction in the injector nozzle and thus the resulting droplet velocity. Mixture formation is also significantly affected by the spray disintegration which predominantly depends on the Weber number and typically ends for Weber numbers below ~ 10 - 12 /27/, /28/. Further reduction of the droplet diameter requires evaporation. Assuming identical conditions of the gaseous phase, the resulting droplet diameter is

proportional to the surface tension and reciprocal proportional to droplet velocity. Increased viscosity may induce higher friction in the nozzle and reduce the droplet velocity. This suggests that 1-Butanol is likely to result in the biggest droplets among the tested fuels while Isooctane is the fuel with the best mechanical and thermo-physical properties for a good mixture formation. Very similar mixture heating values indicate that similar cylinder charges are required to achieve the same power output. The research octane number, although highly relevant for gasoline engine operation, is very difficult to determine for fuels with a high knock resistance and high oxygen content. High enthalpy of vaporization additionally poses problems in the determination of the motor octane number (MON). The European standards for RON and MON determination (DIN EN ISO 5164 and 5163) specify that the accuracy cannot be estimated for gasoline containing more than 4 weight-% oxygen /29/, /30/. DIN 51756-7 contains modifications to allow more accurate measurement of fuels with high alcohol content /31/. Measurements of Ethanol under these boundary conditions have revealed a RON of 108.6 /25/. Taking this into account, one has to be cautious with the octane numbers of 1-Butanol and Tetrahydro-2-methylfuran which were not derived following standard DIN 51756-7.

TEST SET-UP

RESEARCH ENGINE

The engine used in this study is a single cylinder research engine. Injector and spark plug are placed in central cross position in the combustion chamber roof with the spark plug installed between the exhaust valves and the injector being installed between the intake valves, as illustrated by Figure 1.

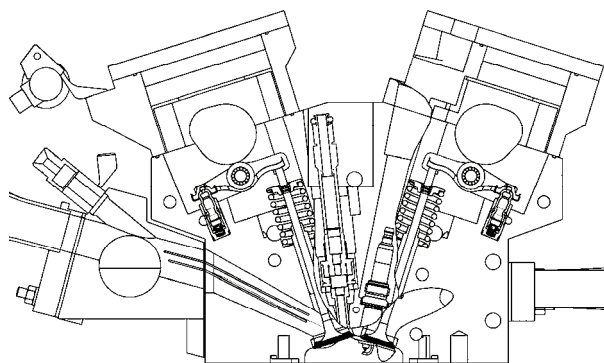


Figure 1: Sectional view of cylinder head

The engine features variable intake and exhaust cam phasing for improved part load efficiency due to internal exhaust gas recirculation strategies. Table 2 gives a summary of the technical data of the test engine. The outward-opening direct-injection gasoline injector has a nominal spray cone angle of $90^\circ \pm 3^\circ$. The maximum needle lift of $\sim 30 \mu\text{m}$ is directly induced by a piezo stack /32/. The high flow rate of $\sim 40 \text{ g/s}$, measured with Isooctane for the injector used within this study, and the short minimal injection

durations allow a high mass flow spread. This covers the different requirements of the investigated fuels caused by the different stoichiometric air requirement. Negative impact on mixture formation caused by too long injection duration at high loads is avoided.

Table 2: Research engine hardware specification

Bore / mm	75
Stroke / mm	82.5
Displacement / cm^3	364
Number of valves / -	4
Max. charging level / bar (abs.)	3.5
Compression ratio / -	In this study: 7 – 13.5
Cylinder peak pressure / bar	170
Fuel injector / -	Continental Piezo
Max. fuel pressure / bar	200

The compression ratio was varied using different pistons. The piston crown design for each compression ratio can be seen in Figure 2.

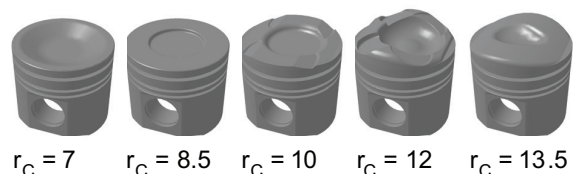


Figure 2: Piston designs

INSTRUMENTATION

The cylinder, intake and exhaust gas pressures are sampled in at least 1° resolution over 200 consecutive engine cycles for the calculation of all indicated values. Higher resolution is used around TDC to enable knock detection. Pressure transducers and thermocouples are used for static pressure and temperature measurements. Oil and water conditioning systems allow steady state operation. The intake air is conditioned to 25°C upstream throttle flap. The pressure up-stream throttle flap and in the exhaust manifold are controlled to 1013 mbar during throttled operation. For charged operation identical pressures upstream throttle flap and in the exhaust manifold are applied to simulate turbocharging. The intake air mass flow is measured with a hot-film air mass meter. Fuel consumption is measured via a volume flow measurement device and also calculated via the measured intake air mass flow and the air excess ratio of the exhaust gas, which in turn is calculated according to the formula derived by Spindt /33/. This is required as fuel metering is not possible for Tetrahydro-2-methylfuran due to its aggressiveness against the materials used in the fuel metering device. The exhaust gas composition is determined from a partial mass flow of exhaust gases which is sampled and fed to the following emission analyzers:

- HC: Flame ionization detector (FID)
- O₂: Paramagnetic oxygen analyzer
- CO: Infrared gas analyzer
- CO₂: Infrared gas analyzer
- NO_x: Chemiluminescence analyzer
- PM: Variable sampling smoke meter
- PN: Condensation particle counter

The response factor of the FID to different HC emissions can result in significant measurement errors, especially for molecules containing oxygen. If the exact HC composition is unknown no corrections of this effect are possible. HC emissions are measured as C₃H₈ for RON95. For all pure fuels the measurement result is recalculated assuming all HC emissions to be the pure fuel molecule itself. Consequently uncertainties on the real HC emissions remain as both assumptions do not reflect the real HC emission spectrum.

TEST PROGRAM

A load variation at stoichiometric air excess ratio from 3 bar to 24 bar indicated mean effective pressure (IMEP) at 2000 1/min in warm conditions is used to study the fuel influence on engine efficiency at different loads and to determine knock sensitivity. In a first phase a compression ratio of 12 is kept constant for all fuels in order to eliminate any potential influences on charge motion, mixture formation and knock sensitivity caused by piston crown design and the compression ratio itself. Limits are defined based on reference measurements with RON95 at a compression ratio of 8.5 in order to allow a determination of the maximum possible compression ratio for each fuel. The first limit is an IMEP standard deviation at full load of 0.37 ± 0.03 bar, indicating unstable combustion that could lead to jerking in the vehicle. The second limit is a centre of combustion of 26 ± 2 °CA ATDC, defined as the point where 50 % mass fraction of the fuel is burned, indicating high knock limitation and decreasing thermal efficiency. Typically combustion stability is linked to the combustion phasing, however, fuel impacts on mixture preparation and combustion can alter the trends typically observed with conventional fuel. Thus both limits are important to compare fuels and define the maximum possible compression ratio for each fuel. Measurements with this individually optimized compression ratio allow first conclusions towards achievable tank-to-wheel efficiency. The fuel influences on homogeneous lean burn combustion systems are studied in two air excess ratio variations at 2280 1/min at a load of 9.4 bar IMEP and at 1500 1/min, 6.8 bar IMEP. All these variations are performed in homogeneous operation mode with single injection into the intake stroke. Spark timing is adjusted for each fuel to keep the centre of combustion constant at 7.5 ± 1 °CA ATDC. The timing is set at the knock limit for operation points where the optimal combustion phasing cannot be realized. The knock limit is defined via the cylinder pressure indication system by the occurrence of combustion cycles with peak to peak knock amplitudes of engine speed divided by 1000 1/(min*bar). A spark timing variation at 1200 1/min and 3 bar IMEP in cold

conditions is used to investigate fuel influences on catalyst heating and cold operation and thus allows a first assessment of tailpipe engine out emissions that can be expected for the different fuels. For this operation mode a double injection strategy is used to improve combustion stability at very late spark timings. This is realized by coupling the end of a short injection with 0.2 ms duration to the spark timing. The delay between the end of this injection and the spark timing was kept constant for all fuels at 5 °CA. All other calibration settings are listed in Table 3.

Table 3: Engine calibration settings

	Load variation	Air excess ratio variation	Spark timing variation
Engine speed / 1/min	2000	2280 1500	1200
Engine load / bar	var.	9.4 6.8	3
Injection pressure / bar	200	200	200
Start of 1st injection / °CA BTDC	300	300	var.
End of 1st injection / °CA BTDC	var.	var.	290
End of 2nd injection / °CA BST	-	-	5
Duration of 2nd injection / ms	-	-	0.2
Intake valve opening at 1 mm / °CA ATDC	10	10	27
Exhaust valve closing at 1 mm / °CA BTDC	10	10	40
Air excess ratio / -	1	var.	1.03
Coolant & oil temperature / °C	90	90	30

RESULTS

LOAD VARIATION

Engine operation at part loads of 3 bar and 6 bar IMEP does not reveal significant differences between the fuels. The center of combustion can be kept identical for all fuels at these two operation points due to the absence of knock. Combustion delay and combustion duration vary only slightly, therefore spark timings, required to achieve optimal combustion phasing, differ only by 2 °CA. This small difference can partly be related to the high charge motion of the engine that diminishes these differences. As a consequence of similar combustion phasing and duration the indicated efficiencies of all fuels are identical within the accuracy of mass flow measurements and heating value determination and result within 29.9 % - 30.8 % for 3 bar and 34.5 % - 35.4 % for 6 bar IMEP, see Figure 3.

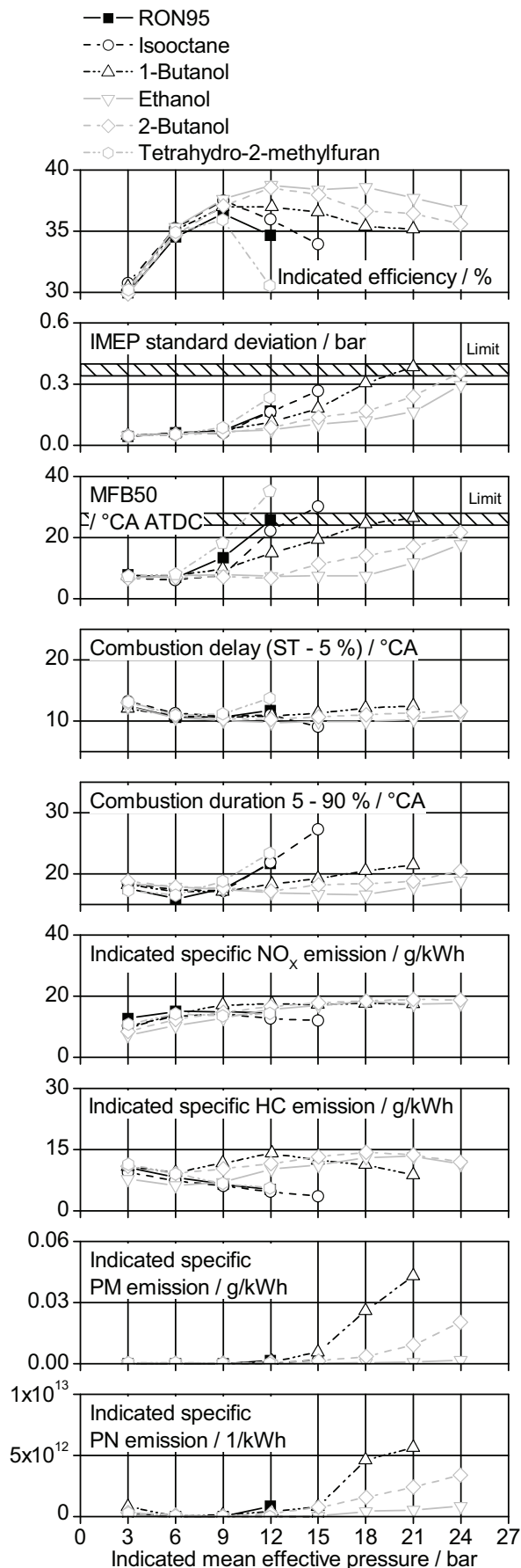


Figure 3: Results of the load variation at 2000 1/min with $r_c = 12$

Raising the load above 6 bar reveals the differences in knock resistance between the fuels. Tetrahydro-2-methylfuran has the lowest knock resistance and the center of combustion has to be retarded the furthest for a given load. This results in the highest combustion delay and combustion duration and a decreased thermal efficiency that becomes pronounced at 12 bar IMEP where the limit for center of combustion is already exceeded by 9 °CA and indicated efficiency drops to 30.5 %. At the same load RON95 exactly reaches the limit for center of combustion with a moderate efficiency drop to 34.7 %. This indicates that a compression ratio significantly below 8.5 is required for Tetrahydro-2-methylfuran in order to achieve 24 bar IMEP within the defined limits. Despite a lower RON, 1-Butanol has a higher knock resistance compared to RON95 and also Isooctane. Still knock limitation at 12 bar IMEP leads to a center of combustion retardation of 7.5 °CA attended by an efficiency loss of ~ 1.5 %-points compared to Ethanol and 2-Butanol which are both not knock limited at this load. 1-Butanol allows a load of 21 bar until the combustion stability and phasing limits are reached, indicating the requirement for a moderate compression ratio reduction to meet the limits at 24 bar. Ethanol is the most knock resistant fuel allowing for a further compression ratio increase as neither the combustion stability nor the limit for center of combustion are exceeded at 24 bar IMEP. The knock resistance of 2-Butanol is slightly lower, thus this fuel exactly meets the combustion stability limit at 24 bar IMEP and compression ratio 12. Both fuels enable the highest indicated efficiency of 38.5 % - 38.8 % at 12 bar IMEP with an ideal phasing of the mass fraction burned. At higher loads Ethanol has benefits versus 2-Butanol of up to 5.3 % with advantages in combustion phasing of up to 6.5 °CA at 18 bar IMEP. The combustion delay and combustion duration typically increase if the center of combustion is retarded due to knock limitation. The only exception is noticeable for Isooctane at 15 bar IMEP where a shorter combustion delay is measured despite the retarded center of combustion. This is caused by an approximately 3 % fuel conversion prior to the spark timing at - 2 °CA BTDC as illustrated in Figure 4 showing the cumulative mass fraction burned and the burn rates of all fuels for a load of 3 bar and 15 bar IMEP. This effect is stable throughout all recorded 200 consecutive cycles and could even be reproduced in another testing campaign with a new fuel batch. Analysis using computational fluid dynamics with a multi-dimensional zone model have revealed that this pre-ignition could be related to the reaction kinetics of Isooctane /34/. The HC emissions are significantly influenced by mixture formation and post oxidation in the exhaust manifold and thus by the exhaust gas temperature. All three alcohol fuels have a higher enthalpy of vaporization compared to the other three fuels. As a consequence the exhaust gas temperatures are lower and HC post oxidation is reduced. This effect is pronounced at higher loads where the superior knock resistance and the resulting advanced combustion phasing is different from the other fuels, see Figure 3. However, the measured increase in HC emissions is more likely caused by