Tailor-Made Fuels from Biomass – Fuels Research to Secure Sustainable Mobility

Tailor-Made Fuels from Biomass – Kraftstoffforschung zur Sicherung nachhaltiger Mobilität

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Abstract

In the Cluster of Excellence Tailor-Made Fuels from Biomass newly derived biogenic fuels are being developed and investigated. Thereby, no limitation is put on the possible fuel candidates with regard to their molecular structure. Based on predicted engine-relevant property data and despite limited experience on auto-ignition of ketonic fuels, ketonic carbonyles were chosen for in-depth investigation in the gasoline engine. Exceptionally good knock resistance and mixture formation at challenging boundary conditions have been experimentally confirmed for 2-butanone, a prototype of a ketonic biofuel comprising tailored properties. To ensure the safe handling of the new fuel candidate its compatibility with seal materials and engine oils has been screened.

1. Introduction

The TMFB fuel design aims at the identification of molecular structures comprising engine-relevant properties and their sustainable production pathways. For this, researchers from the field of chemistry, chemical engineering and mechanical engineering have joined in the Fuel Design group to find the optimum fuel depending on the desired application. As an example of this fuel design, the derivation and investigation of the ketonic compound 2-butanoneis described in this work.

2. Computer-Aided Molecular Design

The first challenge when designing optimal fuel components is the identification of candidates out of the +10.000.000 compounds that could theoretically be derived from lignocellulosic biomass. For this, a tool based on Quantitative Structure-Property Relationships (QSPR) [1, 2]was developed that, in a first step, generates all possible molecular structures based on valance rules and given restriction (e.g. number of carbon atoms) and can then be used to minimize the found data set by user-defined boundary conditions [3]. As in this work it was attempted to find a biomass-based gasoline type fuel, constraints were set, besides other, on the oxygen content, the maximum boiling temperatures and the ignition characteristics expressed by the Derived Cetane Number. As a result, the group of ketones was chosen for further investigations as it is characterized by low boiling temperatures as well as very low self-ignition tendencies, see [3].

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3. Fuel properties

Table 1 lists the most relevant properties of the experimentally studied fuels.

	RON 95	Ethanol	2-Methyl-furan	2-Butanone
Boiling temperature / °C	41.5-173.5	78	64	80
Specific enthalpy of vaporization / $kJ/kg_{air,\ \lambda = 1}$	28.08	101.6	35.52	46.10
Lower heating value / MJ/kg	42.13	26.84	30.37	31.45
Lower heating value / MJ/l	31.05	21.09	25.32	27.63
Stochiometric air requirement / -	14.14	8.98	10.08	10.52
RON MON	96 85	109 90	101 82	117 107

Table 1: Fuel Properties

Ethanol is known as an excellent biofuel for gasoline engines especially at high engine loads due to its high knock resistance and high heat of vaporization. These characteristics enable efficiency improvements of up to ~13 % compared to conventional RON 95 gasoline fuel [4, 5]. Therefore ethanol is defined as the benchmark biofuel for spark ignited engines. However drawbacks arise from the low volumetric heating value and the weak cold start capability. The high heat of vaporization and low vapor pressure in combination with an increased fuel demand due to the lower stoichiometric air requirement lead to a deterioration of mixture formation [6]. Previously performed calculations revealed that for the formation of an ignitable stoichiometric mixture at -30 °C ambient temperature a specific heat of vaporization smaller than 60 kJ/kg_{air} is needed [7].
The engine test bench investigations revealed 2-methylfuran as a potential candidate for a future gasoline fuel [8]. The high vapor pressure and only moderate enthalpy of vaporization lead to a superior mixture formation at cold start conditions compared to ethanol. Efficiency improvement of up to ~10 % compared to conventional RON 95 gasoline fuel can be achieved at full load operation.
2-butanone is a potential biofuel candidate combining a knock resistance significantly higher than 2-methylfuran, a moderate volumetric heating value and a good mixture formation especially at cold start conditions. It is one example of the ketonic fuels structures derived in the computer-aided molecular design.

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4. Experimental Results

The engine test bench investigations were carried out on a homogeneously operated direct injection spark ignition single cylinder research engine known from previous publications [4,8,9]. In contrast to the previously used outward-opening piezo injector, a 6-hole solenoid injector was installed. The achievable thermal efficiency of a gasoline engine predominantly depends on the compression ratio which in turn is limited by the knock resistance of the fuel. Figure 1 depicts the knock resistance in terms of the 50 % mass fraction burned point using a compression ratio of 13.5 at an engine speed of n = 2000 min^{-1} and full load at 27 bar indicated mean effective pressure (IMEP). A 50 % mass fraction burned point (MFB50) at or close to the optimum of 8° CA ATDC indicates a high knock resistance and hence the highest possible engine efficiency. The evaluation of the performance of 2-butanone was conducted by a comparison of measurements under equal boundary conditions for both ethanol and 2-butanone. The full load investigation confirmed the high knock resistance of 2-butanone under real engine conditions.

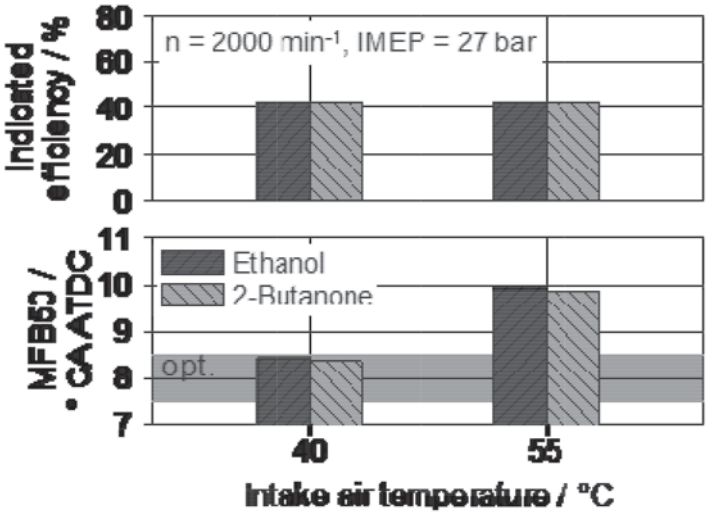

Figure 1: Full load engine test results

For both fuels the intake air temperature had to be raised to 55 °C to exhibit knocking combustion and thus depict the need of combustion phasing (cf. Figure 1). The heating value of 2-butanone was predicted leaving some uncertainty regarding the precision. However the slight difference in efficiency can be explained by the higher heat of vaporization of ethanol and therefore reduced thermal losses.
Figure 2 shows the engine test results at the catalyst heating point. The temperature of the engine fluids was reduced to 40 °C for engine oil and 30 °C for coolant water. For all investigated fuels the spark timing was set to 25° CA ATDC.

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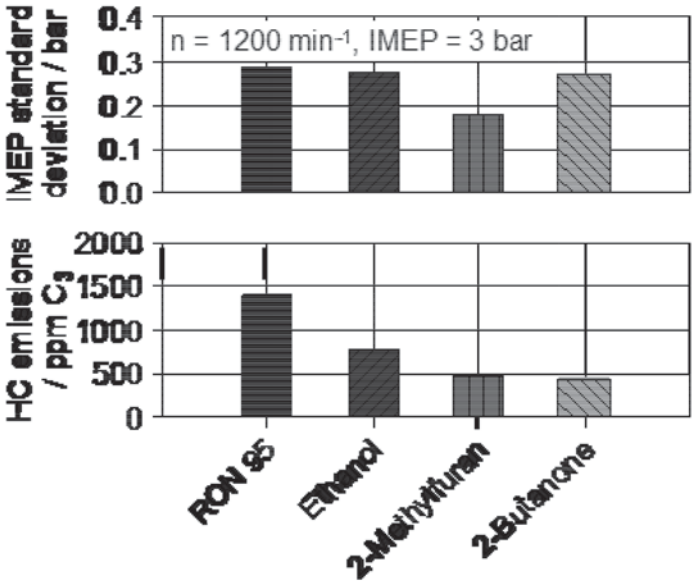

Figure 2: Engine test results at catalyst heating load point

The short burn delay and duration in case of 2-methylfuran result in a good combustion stability of 2-methylfuran indicated by the low standard deviation [9]. For ethanol and 2-butanone a nearly equal cyclic variation is measured. Although the level of HC emissions is partially influenced by the differences in post-oxidation occurring in the exhaust system due to the different temperature level, it can be stated that the low HC emissions of 2-butanone similar to those of 2-methylfuran indicate a good mixture homogenization. Hence the expectation of 2-butanone being a fuel with excellent knock resistance and mixture formation at challenging boundary conditions is experimentally confirmed.

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Zukunft Mobilität – Alternative Energieträger und Antriebe

Wolfgang Steiger

Abstract

Energy and resource efficiency is a political and societal aim. Thisrequires a continuous improvement in conventional powertrain efficiency and the market introduction of electrified vehicles. To result in a remarkable reduction of mobility-related CO_2-emissions, in parallel an energy change for both, conventional hydrocarbons and electric energy, is necessary.

1. Einleitung

Die europäische politische Agenda im Energie- und Verkehrssektor wird maßgeblich durch die Eingrenzung des Treibhausgaseffektes geprägt. CO_2 als einer der Hauptverursacher wird daher stark reglementiert. Als technische Lösungsansätze ergeben sich in der Mobilität zwei komplementäre Strategien:

1. Die Steigerung der Effizienz aller Prozesse in Herstellung und Nutzung von Fahrzeugen, d.h. der reduzierte Einsatz von Energie.
2. Die Dekarbonisierung der genutzten Energieträger, wobei dies aufgrund des globalen Effektes der CO_2-Emissionen auch in der Vorkette, d.h. bei der Herstellung der Energieträger, erzielt werden kann.

In diesem Zusammenhang spielen alternative Kraftstoffe, bzw. Energien, eine entscheidende Rolle. Wichtig ist jedoch nicht nur die CO_2-Bilanz dieser Kraftstoffe, sondern auch deren Anwendbarkeit in heutigen und zukünftigen Antriebssystemen. Bei deren Bewertung ist daher auch eine Vorausschau auf zukünftige Antriebe und deren Rahmenbedingungen notwendig.

2. Zukünftige verbrennungsmotorische Antriebe

In der Automobilindustrie wird seit Jahren die Effizienz der Fahrzeuge kontinuierlich verbessert. So wurde der Kraftstoffverbrauch der Neuwagenflotte seit 1995 um 32% verbessert. Im Mittel werden die Kraftstoffverbräuche bis 2020 um ca. 5% je Jahr weiter reduziert um den Flottenemissionswert von 95 gCO_2/km zu erreichen. Hierzu sind vor allem weitere Verbesserungen in der Antriebseffizienz notwendig. Variable Ventiltriebe und Verdichtung, höhere Einspritzdrücke und verbesserte Verbrennung, Reibungsreduzierung sowie Downspeeding mit größerer Getriebespreizung sind die kommenden Maßnahmen an konventionellen Antrieben.
Diese teils extrem aufwändigen Technologien müssen durch eine entsprechende Verbesserung der Kraftstoffqualität unterstützt werden. Neben der funktionalen Qualität ist aber auch eine Dekarbonisierung notwendig. „Low-hanging-fruits“ wie die verstärkte Nutzung von Erdgas müssen durch neuartige Kraftstoffe ergänzt werden, die

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