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# Tailor-Made Fuels from Biomass: Potentials of 2-butanone and 2-methylfuran in direct injection spark ignition engines

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ABSTRACT

Two possible future biofuels, 2-butanone also referred to as methyl ethyl ketone (MEK) and 2-methylfuran, identified within the Cluster of Excellence "Tailor-Made Fuels from Biomass" (TMFB), have been evaluated as pure fuels in the present study. Investigations of the autoignition tendency were carried out on a rapid compression machine (RCM), whereas thermodynamic investigations were conducted on a direct injection spark ignition single cylinder research engine. 2-Methylfuran and 2-butanone were compared against the present benchmark biofuel for spark ignition engines ethanol and conventional RON95 gasoline. A similar autoignition tendency compared to ethanol was found for 2-methylfuran. In case of 2-butanone very high ignition delay times were measured, even higher than for ethanol and 2-methylfuran. For 2-butanone and 2-methylfuran, the lower heat of vaporization in combination with higher vapor pressure and better primary breakup compared to ethanol are beneficial for mixture formation. During the engine testing for both fuels, superior characteristics compared to conventional gasoline and ethanol were identified. In case of 2-methylfuran, an increased combustion stability, especially at low engine load and cold boundary conditions, could be found at a higher knock resistance than conventional gasoline. In combination with increased compression ratio this enables an efficiency increase of up to 19%, whereas for ethanol an even further increase of up to 21% is possible. 2-Butanone shows increased combustion stability at low engine load and cold boundary conditions compared to ethanol and also conventional gasoline as well as highest knock resistance equal to ethanol. However, for both 2-butanone and 2-methylfuran increased emissions of nitrogen oxides were found when compared to ethanol. For both possible future biofuels and also ethanol, a significant reduction of particle emissions compared to conventional gasoline was found.



## 1. Introduction

The increasing energy demand and the finiteness of the fossil fuels force the transportation industry to seek for alternative energy sources. However, within the upcoming years it cannot be foreseen that a sufficient energy supply for the transport sector can exist without the use of internal combustion engines. At the same time, $CO_2$ emissions are to be reduced to limit the anthropogenic global warming. As liquid fuels based on renewable raw materials (biofuels) hold the promise of closing the carbon cycle, well selected biofuels can supply both a direct $CO_2$ emission reduction due to reduced $CO_2$ in a well-to-wheel evaluation, and an indirect reduction due to the improvement of engine efficiency. In addition, the fuels derived from biomass allow for an increased independence from fossil fuels. Therefore, a variety of possible energy carriers and conversion methods is being investigated by the scientific society. In the Cluster of Excellence "Tailor-Made Fuels from Biomass" (TMFB), newly derived biogenic fuels are being developed and investigated. The TMFB fuel design aims at the identification of molecular structures exhibiting favorable properties for engine application as well as 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. The first challenge when designing optimal fuel components is

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**Nomenclature**

| | |
|---|---|
| $\eta$ | dynamic viscosity of the fluid |
| $\lambda$ | relative air/fuel ratio |
| $\varphi$ | relative fuel/air ratio |
| $\rho$ | density of the fluid |
| $\sigma$ | surface tension of the fluid |
| $\tau$ | ignition delay time |
| $\tau$ | ignition delay time measured through an experiment |
| $c_p$ | specific heat capacity |
| $d$ | characteristic length |
| $\Delta h_v$ | enthalpy of vaporization |
| $r_c$ | compression ratio |
| $v$ | velocity of the fluid relative to ambient conditions |
| $p$ | pressure |
| $T$ | temperature |
| $R$ | universal gas constant |
| ATDC | after top dead center |
| BTDC | before top dead center |
| CA | crank angle |
| CO | carbon monoxide |
| $CO_2$ | carbon dioxide |
| DI | direct injection |
| $D_p$ | mobility particle diameter |
| EVC | exhaust valve closing (1 mm) |
| EVO | exhaust valve opening (1 mm) |
| FSN | filter smoke number |
| HC | hydrocarbon |
| IMEP | net indicated mean effective pressure (calculated over 720° CA) |
| IVC | intake valve closing (1 mm) |
| IVO | intake valve opening (1 mm) |
| KLSA | knock-limited-spark-advance |
| MEK | methyl ethyl ketone(2-butanone) |
| MFB 50 | point where 50% mass fraction of the fuel is burned |
| MON | motor octane number |
| $NO_X$ | oxides of nitrogen |
| NTC | negative temperature coefficient |
| *Oh* | Ohnesorge number |
| PN | particulate number |
| PRF | primary reference fuel |
| QSPR | quantitative structure–property relationships |
| *Re* | Reynolds number |
| RON | research octane number |
| SI | spark ignition |
| SOI | start of injection |
| ST | spark timing |
| TDC | top dead center |
| TMFB | Tailor-Made Fuels from Biomass |
| TPA | three pressure analysis |
| *We* | Weber number |

the identification of candidates out of the more than 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, which initially 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]. A low auto-ignition tendency, a heating value >30 MJ/kg, a boiling point between 50 and 100 °C and an enthalpy of vaporization <60 kJ/kg was selected as combustion system depending requirements for spark ignition engines. In this paper, the potentials of two possible biofuels, identified by the fuel design process [2,3] of the TMFB Cluster for the use in spark ignition engines, are evaluated by theoretical assessments and experimental testing in both a rapid compression machine (RCM) and a single cylinder research engine. Thewes et al. [4,5] already presented 2-methylfuran as a promising fuel candidate for future high efficient spark ignition engines. Additional investigations on this fuel and investigations on the recently identified 2-butanone will be presented in this paper. For both fuels, possible pathways for the production from biomass have been identified [6–10]. The focus of this publication is to investigate the influence of the pure fuel molecules on the combustion behavior by avoiding cross influences of the conventional gasoline in blended fuels.

## 2. Materials and methods

### 2.1. Rapid compression machine

The RCM used during the course of this study has been described in detail by Lee et al. [11]. Briefly, it has a single piston configuration, with a variable volumetric ratio, which is possible through the interchange of the end walls altering the ratio of the volumes before and after compression. This option allows the user to access different compressed temperature and pressure conditions, while studying the same mixture. The RCM is equipped with a heating system covering the reactor chamber, which is controlled and monitored by 13 thermocouples spaced axially along the reactor chamber. This method ensures a homogeneous initial temperature and also allows the RCM to study various initial temperatures (ambient up to 423 K). The ability to operate the RCM at different initial temperatures is specifically important when studying non-volatile fuels with low vapor pressures. The facility was heated to 343 K for this study. This temperature ensured that the liquid fuel was in the gaseous phase throughout testing. Creviced piston heads were used in order to suppress the formation of roll-up vortices, thereby ensuring a homogenous temperature field within the reactor core at the end of compression.

The RCM has an estimated uncertainty of 20% in the measured ignition delay times. At each compressed temperature, ignition delay times were measured in duplicate to ensure repeatability in the measurements. The pressure within the RCM was measured using a recessed and silicon coated PCB113B24 sensor. The compressed conditions were calculated using the compression/expansion routine in the Gaseq code [12]. This assumes frozen chemistry during compression, which is an adequate assumption due to the rapid compression associated with this RCM.

Fig. 1 presents a typical pressure trace obtained during the measurement of the ignition delay times presented here. Also highlighted in Fig. 1 is the definition used for ignition delay time in all experiments.

Ignition delay time ($\tau_{ign}$) was defined as the time between the end of compression (time = 0, when the piston has come to its end of stroke position) and the near instantaneous pressure increase caused by ignition. All experiments reported showed a nearly instantaneous pressure increase defining ignition similar to the example in Fig. 1. 2-Butanone was supplied by Sigma–Aldrich (⩾99.0%). Westfalen AG and Praxair supplied oxygen (⩾99.995%), argon (⩾99.996%) and nitrogen (⩾99.95%). Mixtures were premixed in two 1 l stainless steel heated mixing vessels. The mixtures were allowed to mix for at least 30 min in order to ensure a homogenous mixing via gaseous diffusion.