

# Optimization of Diesel Combustion and Emissions with Tailor-Made Fuels from Biomass

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## ABSTRACT

In order to thoroughly investigate and improve the path from biofuel production to combustion, the Cluster of Excellence “Tailor-Made Fuels from Biomass” was installed at RWTH Aachen University in 2007. Since then, a variety of fuel candidates have been investigated. In particular, 2-methyl tetrahydrofuran (2-MTHF) has shown excellent performance w.r.t. the particulate (PM) / NO<sub>x</sub> trade-off [1]. Unfortunately, the long ignition delay results in increased HC-, CO- and noise emissions.

To overcome this problem, the addition of di-n-butylether (DNBE, CN ~ 100) to 2-MTHF was analyzed. By blending these two in different volumetric shares, the effects of the different mixture formation and combustion characteristics, especially on the HC-, CO- and noise emissions, have been carefully analyzed. In addition, the overall emission performance has been compared to EN590 diesel.

The results show that an addition of DNBE to 2-MTHF can lead to a reduction of HC- and CO-emissions by 75 % and noise emissions up to 4 dB. Simultaneously, none of the benefits gained with 2-MTHF with regard to the PM-emissions are not sacrificed. It could be proven, that by blending two molecules that are derived from biomass, a tailor-made fuel can be designed that allows optimizing the diesel combustion according to the desired criteria.

In addition, both fuels were investigated in a High Pressure Chamber (HPC). Based on the results, new characteristic fuel numbers shall be developed in order to describe the combustion behaviour of the new fuels in a proper way, since the established ones are not sufficient to describe the combustion and emission performance of these fuels.

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## INTRODUCTION

In order to promote fundamental research at German universities, in 2006 the “Excellence Initiative” was instituted by the German Research Foundation. Since then, a variety of so called “Cluster of Excellence” was installed at German universities, carrying out fundamental research in almost all subject areas. The Cluster of Excellence “Tailor-Made Fuels from Biomass” (TMFB) at RWTH Aachen University was established in 2007 as part of this initiative in order to undertake fundamental research on new, biomass-based, synthetic fuels for use in vehicle applications. For this purpose, 21 institutes from the RWTH, as well as two external research institutions (Fraunhofer Institute for Molecular Biology and Applied Ecology, Aachen and the

Max-Planck Institute for Coal Research, Mülheim) from the fields Biology, Chemistry, Process Engineering, and Combustion Engineering have clustered in the “Fuel Design Center”. The long-term objective of this Cluster of Excellence is to determine the best possible combination of fuel components, whose properties will be determined by the requirements of future combustion processes. The vision of the Cluster of Excellence is to develop the entire process chain for a novel tailor-made fuel from biomass to the combustion engine, without creating competition to the food chain.

By the research undertaken in the past 5 years, a variety of possible, future fuel candidates have been developed. Since most of the derived molecules differ significantly in their chemical composition and molecular structure, from

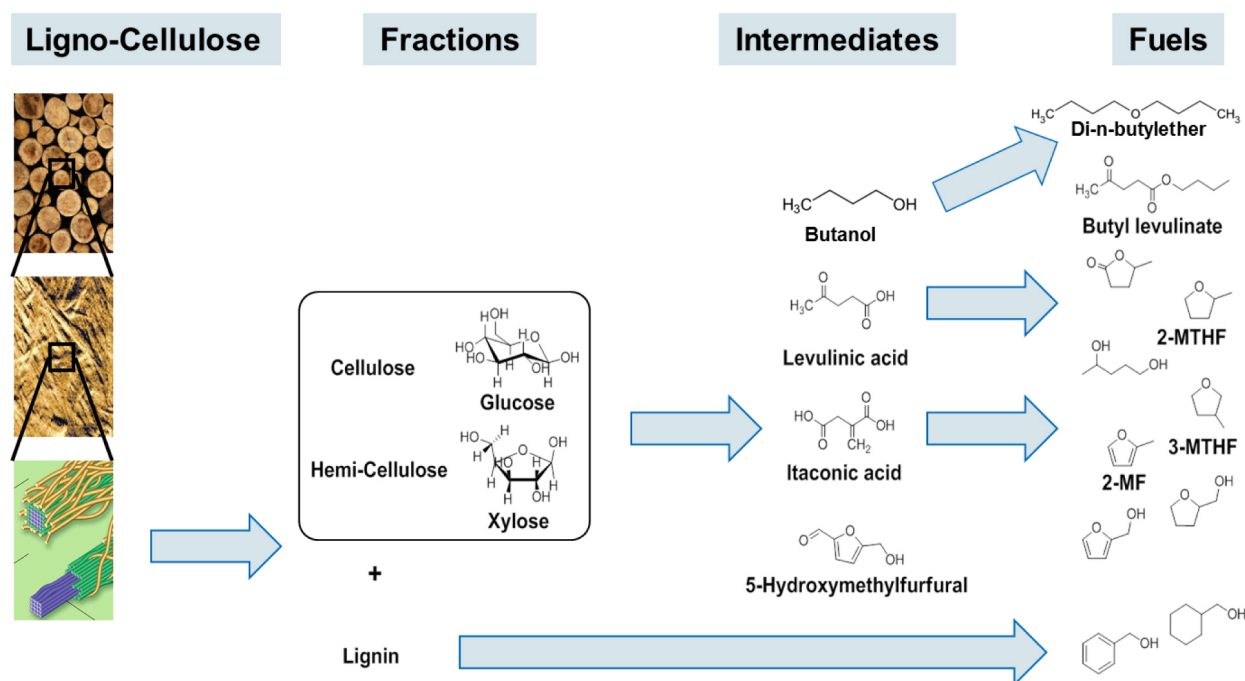


Figure 1. Production routes of TMFB [9]

conventional fossil fuels, new characteristic fuel numbers are being developed describing the combustion behavior beyond the information that established numbers, e.g. cetane number, are able to deliver. This fundamental research is undertaken using different facilities. For example, an indicator for air/fuel mixture quality prior to ignition, the “Overlap Number” (OLN) has been established based on measurements in the High Pressure Chamber [2, 3].

More recently, gasoline as well as diesel candidate fuels have been developed, allowing an optimization of the corresponding combustion behavior. Nevertheless, as specific fuel properties have mainly positive effects on the final combustion and emission behavior - for example a high oxygen content decreases particulate emissions -, not all emissions can be decreased simultaneously. In general, a longer ignition delay leads to a good mixture preparation and therefore low soot emissions, but elevated HC- and CO emissions are usually detected at the same time. For instance, 2-MTHF has been considered as a tailor-made biofuel for passenger car diesel engines because it allows nearly soot-free combustion in a diesel engine, even at the lowest engine-out NO<sub>x</sub> levels [4,5,6]. Since the vapour pressure of 2-MTHF is rather high and in parallel the air/fuel mixture is of low reactivity, the HC- and CO-emissions exceed those of conventional diesel by factor of about two due to over-leaning effects [1]. Thus, the aim of this work is to analyze different mixtures of two tailor-made fuels from biomass, one with a very low cetane number of only 15 (2-MTHF) and the other one with a higher cetane rating of 100 (di-n-butylether). The adjusted combination of both components is aimed to minimize the above mentioned effects of long ignition delays

while maintaining the high potential to decrease particulate emissions.

## PRODUCTION PATHWAYS OF TAILOR-MADE FUELS FROM BIOMASS

Presently available biofuels are produced in the following manner: for diesel application, vegetable oils are esterified to make biodiesel (B100), while for gasoline-like fuels, starches as well as sugars are fermented into bioethanol. However, cultivating crops for the production fuel stands in direct competition with the necessity of growing food and feed plants (e.g. [7]). Furthermore, in the described biodiesel and bioethanol production processes, only the fruit and seeds of the plants are being used. In order to increase the yield per area, future concepts target the complete utilization of plant material that is not used as a food source. The work of the cluster of excellence TMFB also aims for using non-food-chain competitive biomass as origin for the developed fuels. In general, biomass consists of lignocellulose. This is a complex composite material made up of three biopolymers: cellulose, hemicellulose, and lignin. Within TMFB, the production pathways for the tailor-made fuels rely on the selective (bio-) chemical transformation processes of lignocellulosic biomass, retaining nature's synthetic effort to the extent possible. To do so, methods are developed for the selective and effective chemical conversion of biomass. First of all, the lignocellulose must be split up into its components cellulose, hemicellulose, and lignin. Innovative reaction media such as ionic liquids are used to break the bonds

between these components and to separate the respective fractions. Ionic liquids are compounds that - such as table salt - are made up of positively and negatively charged ions, have a melting point of below 100 °C and a very low vapor pressure. Using various catalytic conversion methods, the individual components can then be converted into the desired fuel molecules. [Figure 1](#) shows possible methods of converting the lignocellulose fractions via selected intermediates into the desired fuel components.

From the figure it is clear that, depending on the chosen pathway and the targeted intermediate/platform molecule, a large variety of different fuel compounds can be produced from cellulosic biomass with a high selectivity. 2-MTHF can be produced catalytically via reduction and dehydration of levulinic acid [8], while di-nbutylether can be synthesized via etherification of n-butanol.

## DESIRED FUEL PROPERTIES FOR DIESEL COMBUSTION

Within the Cluster of Excellence, a fuel design process has been developed, which incorporates both the scientific progress of the fuel production and the fuel's application. The process as such is highly iterative as well as interactive: Newly-developed fuel molecules provided by the chemical/catalytic members of the fuel design group are methodically investigated and screened with regard to their combustion/application properties for the experiments undertaken. Based on the obtained results, the desired property definition can be updated or changed. One major aim is to structure the experimentally-derived results so that the effect of specific molecular groups or compositions on a specific fuel property can be formulated. By doing this, more general statements and optimization criteria can be formulated when experimental feedback is given to the fuel production side. [Figure 2](#) displays the iterative nature of the fuel design process, serving as a coupling element between fuel production and use. [9]

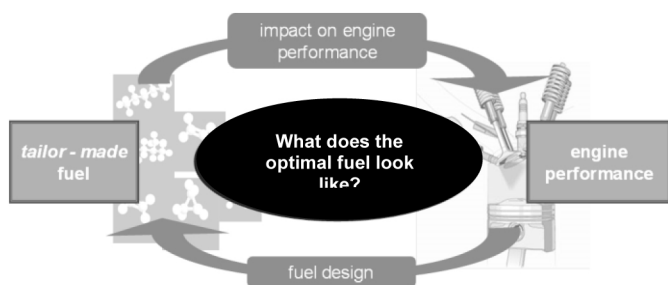


**Figure 2. Schematics of the Fuel Design Process**

In order to define a proper starting point for the molecules to be investigated within this iterative fuel design process, well-known alkanes, alcohols and esters have been characterized in an initial step, to gain fundamental understanding of the effect of a molecules structure on the combustion characteristics. For determining the chemical

reaction kinetics of the molecules, a **Shock Tube** as well as a **Rapid Compression Machine** (RCM) is utilized within the Cluster of Excellence. Both facilities require homogenous mixtures, but whereas the Shock Tube is able to investigate high temperature kinetics (> 900 K), the RCM is used for measuring the ignition delay in the low- to medium-temperature regime (700 - 900 K). In particular for modern diesel combustion engines with high rates of recirculated exhaust gas (EGR) and therefore lower temperatures of combustion, this is the relevant temperature range for ignition. In order to thoroughly investigate the spray breakup and evaporation behavior leading up to ignition and soot formation tendency, a **High Pressure Chamber** (HPC, see next main section) was installed at the Institute for Combustion Engines. The HPC features various optical accesses. With inert boundary conditions in the chamber, the main focus is on the spray breakup, the droplet formation and the fuel/air entrainment. On the other hand at engine-like boundary conditions (high temperatures and pressures, pure air) the self-ignition as well as the soot formation in the fuel spray can be analyzed.

**Single-cylinder engines** (SCE) are available for diesel and gasoline investigations, for both purely thermodynamic measurements as well as optical accessible experiments. The thermodynamic measurements aim to characterize the real-operation combustion efficiency and emission-formation tendency of the analyzed fuels. The optically accessible engines allow observation of the mixture formation quality in the cylinder. Also, the temporal path of ignition and emissions formation (especially soot) can be characterized. The specifications of the HPC and thermodynamic diesel SCE are described in more detail in the next section.

All experiments are accompanied by simulation approaches. The results from the shock-tube and the RCM form the basis for combustion kinetic mechanism development. With the optical spray breakup measurements, new Computational Fluid Dynamics (CFD) models are being developed and existing ones are constantly updated as new fuel properties can be integrated into the code. Also, the in-cylinder combustion is being simulated with commercial CFD tools to better understand the phenomena that affect emission formation.

With the introduced measurements, the influence of single specific properties of the fuels could be determined. The characteristics that were found to have a major impact on combustion and emissions are introduced in the following section.

## Relevant Fuel Properties

The fuel properties have a great impact on the complete mixture process of fuel and air. The physical spray breakup, the formation of fuel droplets and the subsequent interaction with the surrounding air, and evaporation of the fuel droplets can be directly related to the physical characteristics of the applied fuel molecules. Second, the combustion kinetics, describing both ignition as well as pollutant formation

chemistry, are also heavily influenced by the chemical composition of the fuel and its molecular structure.

In [Figure 3](#), the fuel properties most relevant for engine combustion are summarized. A classification based on the chemical, physical or “engine-relevant” nature of each specific property is possible but not unambiguous, as no distinct lines can be drawn between the single classes. Obviously, all physical and “engine-relevant” parameters can be traced to the chemical characteristics. Also, the efforts that need to be taken in order to determine each property vary notably from point to point. While the molecular characterization can easily be done with very small quantities and state-of-the-art laboratory equipment, the measurement of combustion-relevant properties like the burning velocity or even the cetane and octane number requires much more effort and sample quantity.

The classification undertaken in [Figure 3](#) reveals another challenge of the interdisciplinary fuel design process that has to be addressed in the development of completely new fuel molecules: while chemists can easily describe the basic chemical properties of a fuel and engineers at the same time are able to define self-ignition criteria of the desired fuel, the characteristics cannot be translated into one another directly. Therefore, it is necessary to bridge the gap between the different classes displayed in [Figure 3](#) and allow for a conversion of engine-related properties into basic physical and then molecular properties and vice-versa. Therefore, model-based methods have proven to bear a great potential, as they allow application of experimental data that was collected with a limited amount of samples to additional, not-yet-analyzed molecular components. [9]

Further, based on these experiments, new characteristic fuel numbers are derived in order to better describe the fuel's behavior and emission potential in internal combustion processes. For instance, only relying on the CN is insufficient for describing the ignition behavior of a fuel. Depending on the in-cylinder conditions, a pure component may show pronounced Negative Temperature Coefficient (NTC) behavior, which is not the case for conventional diesel fuel. In order to describe the soot formation tendency of a fuel, the first step is the development of the “Engine Ignition Delay Time” (IDN) and the “Overlap Number” (OLN, see next chapter) as described by Janssen et al. [20]. Both numbers can be utilized to qualitatively rate the soot formation tendency of a fuel, since they describe the time for mixture formation before ignition, which will be discussed in more detail in the following sections.

As mentioned, the desired fuel characteristics have been revealed by carrying out not only engine experiments, but also fundamental experiments such as optical injection investigations, ignition delay measurements with an RCM and HPC, as well as basic experiments on the emission-formation potential of the molecules like smoke point measurements. Combining the results of these experiments conducted, it becomes possible to individually assess the influence of the molecular composition of the fuel molecules

on the combustion behavior and, in the next step, formulate desired properties as to how an optimized fuel should look. Based on the experiments undertaken, an optimized biofuel for diesel combustion was characterized as follows [6]:

- Long - but limited - ignition delay for good mixing and, at the same time, cold-start operation.
- Oxygen content ranging from 10 to 25%. Smoke Point measurements indicate that this percentage is sufficient to have a notable soot reduction effect [10].
- Low boiling point with a minimized surface tension to enhance spray breakup and mixing.

The definition of these demands led to the development of 2-MTHF (see [Figure 1](#)) as a promising candidate for diesel combustion [1]. Due to its low self-ignitability and the high oxygen content, the typical PM / NO<sub>x</sub> trade-off could almost be eliminated, even in high load points. The drawback of the long ignition delay and the reduced self-ignitability is the increased HC- and CO-emissions as well as poor combustion stability, in particular at low load operation. To overcome these problems, an “ignition booster” has been identified within the fuel design process: via etherification of biomass-based n-butanol, di-nbutylether can be synthesized. This molecule provides a sufficient oxygen content as well as a very high cetane number (~ 100) [11]. Thus, this molecule should be an adequate blending component for improving combustion behavior particularly at low load-operation. Initial results with a mixture of 70% 2-MTHF and 30% DNBE have indicated the potential to decrease HC and CO emissions while maintaining soot-free combustion [12, 13].

Unfortunately, particularly 2-MTHF is a rather aggressive fluid compared to diesel fuel. Therefore, all seals at the test benches being in contact with the newly developed fuels have been replaced with seals made of polytetrafluorethylen (PTFE) and all fuel lines are made of either stainless steel or PTFE.

## RESEARCH METHODOLOGY

To assess the potential of the research approach, 2-MTHF and DNBE were investigated in the HPC as well as in a single-cylinder diesel research engine. Starting with 100 % 2-MTHF and DNBE, blends with 20, 30 and 50% vol.-% of DNBE were investigated in the SCE to investigate the possibility of tailoring the combustion characteristics by changing the fuel's properties. For reference, EN590 diesel fuel was measured under the same operating and boundary conditions on both test benches. The general fuel properties of the pure components are depicted in [Table 1](#) on the next page.