



# Influence of fuel properties on fundamental spray characteristics and soot emissions using different tailor-made fuels from biomass



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## ABSTRACT

This work evaluates the potential of some new biomass-derived fuels as candidates for compression ignition operation. Thus, fundamental spray characteristics related to fuel vaporization and fuel/air mixing process for 2-Methyltetrahydrofuran, Di-n-butyl ether and 1-octanol has been studied and compared with conventional EN590 Diesel fuel. For this purpose, OH\* chemiluminescence and shadowgraphy measurements in a high pressure chamber as well as 1D simulations with a spray model have been carried out at different operating conditions representative of the NEDC driving cycle. Finally, measured soot emissions in the single-cylinder engine were presented and discussed.

Results from the high pressure chamber presented very good agreement in terms of liquid length and vapor penetration with simulation results. Thus, some analytical expressions related to macroscopic spray characteristics have been proposed and validated experimentally for all four fuels. Finally, the single-cylinder engine results confirmed the relevant role of soot formation on final emissions for 1-octanol and 2-MTHF. In addition, DNBE showed greater soot oxidation potential than diesel and other TMFB candidates.

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## 1. Introduction

The extensive use of internal combustion engines (ICE) to cover fundamental requirements such as people and goods transportation and power generation has result in their mass production [1]. In spite of their potential, it is well-known that conventional mixing-controlled diesel combustion in compression ignition (CI) engines results in unacceptable raw NO<sub>x</sub> and soot emissions [2–4]. Thus, complex and costly aftertreatment devices are needed to meet the targets imposed by the current emissions regulations [5,6]. This fact, together with the finite nature and instability of fossil fuel supply [7–10], has led to extensive research on alternative fuels which shall contribute to modern combustion systems to reduce both engine emissions and the dependence of ICEs on fossil fuels [11]. In this sense, an imperative long-term goal for the

scientific community is to determine the optimal combination of fuel production processes based on renewable raw materials and their utilization in optimized ICEs.

The use of oxygenated fuel compounds has shown a positive impact on engine-out emissions from conventional mixing-controlled combustion. Recent studies demonstrated that biodiesel fuel allows a consistent reduction of particulate matter (PM) emissions versus conventional diesel [12]. The analysis of spray mixing, vaporization and combustion processes of biodiesel fuel in optical research engines and combustion test rigs allowed to explain the main reasons of the soot emissions reduction [13]. In particular, it was found that because of fuel oxygenation, mixtures are less fuel rich at the center of the jet for biodiesel. Consequently, pre-mixed combustion occurs at lower stoichiometry, closer to the jet center, and confined by a more narrow diffusion flame. The longer time for soot inception and growth, combined with entrained oxygen during this period, ultimately limits the soot formation significantly for biodiesel compared to diesel [14].

More recently, several oxygenated fuels derived from biomass have been identified to be suitable for CI operation. In particular, Decanol has been widely studied in a single-cylinder research engine under conventional mixing-controlled combustion conditions showing up to 90% reduced soot emissions than diesel fuel

*Abbreviations:* 1D, one dimensional; 2-MTHF, 2-Methyltetrahydrofuran; CO, carbon monoxide; DNBE, Di-n-butyl ether; HC, hydrocarbon; HPC, high pressure chamber; ID, ignition delay; IMEP, indicated mean effective pressure; LL, liquid length; LOL, lift-off length; SCE, single cylinder engine; SOC, start of combustion; TMFB, tailor-made fuels from biomass.

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depending on the engine load point [15]. Moreover, the influence of several oxygenated fuels on homogeneous direct injection combustion were investigated using 2-Methyltetrahydrofuran (2-MTHF), 1-Butanol and 2-Butanol [16]. In this case, results showed that these fuels do not provide significant improvements for homogeneous lean burn combustion despite a significant reduction in NOx emissions. The major difference found between these fuels was the knock resistance, which allowed increased thermal efficiency with 2-Butanol through the increase in compression ratio. In addition to the already mentioned fuels, some other biomass-derived components such as Di-n-butyl ether (DNBE) and 1-octanol were also identified as promising candidates for CI operation [17,18]. These fuel candidates feature a high oxygen content together with a rather low boiling point compared to Diesel fuel, which has been shown as a promising way to contribute to a significant reduction in engine-out smoke at various load and speed conditions even with lower engine-out NOx emissions [19–21].

Aside from experimentation, one-dimensional (1D) spray models have been quite often used for the prediction of free spray evolution under steady boundary conditions. Due to the low computational requirements, local flow thermodynamics can be calculated with very high detail, which enables different approaches for the spray analysis. In 2008, Pastor et al. [22,23] presented a 1D model with a general formulation that enables the prediction of any type of spray flow, under both inert and reacting conditions. Furthermore, due to the mixing-controlled hypothesis upon which the model is based, it can be used for the description of both a gas jet and also a diesel spray working under real engine conditions. By making some assumptions derived from the theory of turbulent gas jets, the model enables the estimation of the distribution of properties within the spray (composition, temperature, density, etc.), as well as the tip penetration. This model has been used in literature for complementing studies developed in combustion vessels [24], optical engines [25] and single-cylinder research engines [26]. In 2009, Musculus and Kattke [27] also proposed a 1D model for transient diesel jet with the aim to understand the jet mixing process in case of unsteady injection rate. This was an extension of the Naber and Siebers model and some simplifying assumptions were made based on experimental observations [28]. The model results allowed explaining the formation of fuel-lean regions near the injector after the end of injection (EOI). Moreover, the model indicated the presence of an “entrainment wave” that travels along the jet from upstream, promoting fuel air mixing after EOI. This model has been also used to explain results obtained by means of combustion vessels [14] and optical single-cylinder research engine [29,30].

The main objective of the present research is to study the mixture formation of several fuels derived from biomass, 2-MTHF, DNBE and 1-octanol, to gain understanding on the mechanisms for their low soot emissions. For this purpose, fundamental spray characteristics such as liquid length (LL) and lift-off length (LOL) have been determined by applying simultaneous measurements of OH\* chemiluminescence and shadowgraphy in a high pressure chamber (HPC). Moreover, the 1D spray model proposed by Pastor et al. has been used to complement the experimental information. Finally, in order to validate the findings extracted from the fundamental study under realistic conditions, several soot measurements using a single-cylinder engine (SCE) are presented.

## 2. Experimental facility

### 2.1. High pressure chamber

The optical measurements are conducted at a continuously scavenged HPC test-bench [31]. During operation, a constant air

volume-flow of  $V = 50 \text{ m}_n^3/\text{h}$  (where the subscript  $n$  stands for normal conditions) enters the HPC from the bottom side with a maximum pressure of  $P_{\text{max}} = 140 \text{ bar}$ . Since the resulting air velocity inside the vessel is below  $0.1 \text{ m/s}$ , no significant influence on combustion process is expected. This flow is heated by two electrical cartridges connected in series in the lower test-bench section before entering the measurement volume. Therefore, maximum steady-state temperatures of  $T_{\text{max}} = 1000 \text{ K}$  can be generated, which allows the simulation of a wide range of boundary conditions inside the measurement volume. This volume is accessible by all four horizontal sides. One of these accesses is occupied by the mounted injector, while the three other sides of the measurement volume are equipped with 120 mm silica windows. Therefore, simultaneous optical techniques can be applied in the HPC test-bench. After flowing through the chamber, the air is cooled down, depressurized, and guided through an exhaust after-treatment system.

### 2.2. Injection system

The injection system used a series production piezo-actuated injector equipped with an equiangular 3-hole nozzle. This nozzle design is used to avoid optical overlay of neighboring spray cones from a side view. The main characteristics of the nozzle hole geometry are depicted in Table 1.

The injector is energized by a power-unit with a pull-in current set to 17 A for 300  $\mu\text{s}$ , and holding current set to 12 A. Moreover, the hydraulic delay of the injector, which was determined by light scattering and rate measurements, is 360  $\mu\text{s}$ . In addition, the fuel is pressurized using a piston pump, and the injector is connected to the rail via 2 m long high pressure tube. Furthermore a piezoresistive high pressure sensor (0–2000 bar) is mounted close to the injector.

### 2.3. Fuels

In general, biomass consists of lignocellulose, what is a complex of the three biopolymers cellulose, hemicellulose, and lignin. Within the Aachen-based research group, the production pathways for the tailor-made fuels from biomass (TMFB) rely on the selective (bio-) chemical transformation processes of lignocellulosic biomass, retaining nature's synthetic effort to the extent possible. Therefore, several pathways are developed for the selective and effective chemical conversion of biomass. In a first step, the lignocellulose is split up into its components. In succession, innovative reaction media such as ionic liquids are used to break up the linkages between these components and to separate the respective fractions. Then, the individual components can be converted into the desired fuel molecules using various catalytic conversion methods. In this sense, Fig. 1 shows possible methods of converting the lignocellulose fractions via selected intermediates into the desired fuel components. 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. Thus, DNBE can be synthesized via etherifi-

**Table 1**  
Details of nozzle configuration.

Parameter	Value
Nozzle type	Mini sac
Number of holes	3 (120° spacing)
Orifice diameter ( $\mu\text{m}$ )	118
ks-factor	1.3
Cone angle (°)	148

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