



Di-*n*-buthylether, *n*-octanol, and *n*-octane as fuel candidates for diesel engine combustion



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ABSTRACT

In this study, three different C₈ fuels, namely *n*-octanol, di-*n*-buthylether (DnBE), and *n*-octane, are investigated with regard to diesel engine combustion to assess and analyze the effects of fuel structure. DnBE and *n*-octanol are isomers, i.e. they have the same elementary composition (C₈H₁₈O), but a different structure and very different chemical and physical properties. The ignition behavior of these fuels in engine-like configurations is studied in terms of chemical modeling using recently published detailed kinetic mechanisms. The reduced and enhanced homogeneous ignition propensity of the alcohol and ether functional groups, respectively, are explained by reaction pathway analysis. However, the difference in low temperature reactivity of *n*-octanol and *n*-octane is relatively small compared to the difference in their cetane ratings. To study the engine behavior of these fuels, experiments and simulations were performed. A single cylinder diesel engine was operated with DnBE, *n*-octanol, and *n*-octane as single component fuels. For all three fuels, very low soot emissions at nitrogen oxide emissions within the Euro 6 regulation limits can be reached. Combustion and pollutant formation in the diesel engine are computed using the representative interactive flamelet approach. Results from the numerical simulations show good agreement with the experimental diesel engine tests. A subsequent analysis of the diesel engine simulation results shows that the differences in engine operation and carbon monoxide emissions can be attributed to the different ignitability, reflected by the different cetane ratings of the fuels. The substantially lower cetane rating of *n*-octanol compared to *n*-octane is explained by analysis of engine simulations and homogeneous reactor calculations. The effect of the different physical fuel properties does not play a significant role in the operation range studied. However, it is found that one of the main reasons for the large differences in cetane numbers between *n*-octane and *n*-octanol is the different stoichiometric mixture fraction, which leads in diesel engines to lower temperatures at the ignition location and hence to longer ignition delay times.

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1. Introduction

Future needs for continuous mobility motivate the search for alternatives replacing fossil energy sources. One attractive option for this is the production and use of fuels from biomass, which have the potential to reduce pollutant emissions such as soot or nitrogen oxides (NO_x) considerably. First generation biofuels, e. g. ethanol and bio-diesel, have been successfully applied in the transport sector during the past few years. However, as a drawback, the production of these biofuels is in general in competition with food supply and can lead to increasing cost for food. Nowadays, second generation biofuels, whose feedstocks exclude food crops, have attracted worldwide

attention of research communities. One of the possible resources is lignocellulosic biomass, e. g. waste biomass or high-yielding energy crops. From lignocellulose, ethanol can be directly produced by hexose fermentation. While ethanol has been widely used as a bio-fuel additive for gasoline, its application in diesel engines is limited due to its ignition quality. Recently, two isomers, *n*-octanol and di-*n*-buthylether, have been identified as biofuel candidates [1,2] for diesel engines from lignocellulosic platform chemicals. The linear primary *n*-octanol can be obtained through a highly selective catalytic synthesis from biomass-derived furfural and acetone [1]. In addition, DnBE can be obtained by the dehydration of *n*-butanol [3], which is the product of the further conversion from ethanol.

The holistic development of these second generation biofuels as a combination of biomass processing and combustion technology has proven to be a research area with a high need for interdisciplinary cooperation between natural and engineering sciences. From the combustion engineering perspective, it is of primary interest to

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understand the interdependencies of fuel molecular structure and oxidation performance in detail. Cai et al. [4] studied the oxidation of DnBE experimentally and numerically. The ignition delay times and the burning velocities were measured in a laminar flow reactor and a stagnation flame configuration, respectively. A chemical mechanism was developed to describe these global combustion properties and to elucidate the reaction pathway of DnBE at various conditions. *n*-octanol oxidation was investigated in a high pressure shock tube and in a jet stirred reactor [5]. The ignition delay times of *n*-octanol were computed with the derived reaction mechanism and compared to those of the linear alkane, *n*-octane. In comparison to the linear alkane with the same carbon number, the alcohol and ether functional groups in the molecular structure were found to reduce and enhance homogeneous ignition propensity of fuels, respectively [4,5]. However, the inhibitory effect of the alcohol functional group on the fuel reactivity is reduced for *n*-octanol compared to alcohols with lower carbon chain length.

In addition to the chemical kinetic studies mentioned above, several engine experiments were conducted for DnBE and *n*-octanol in the past [6–8]. Beatrice et al. [6] and Heuser et al. [7] tested DnBE as a pure fuel and as an additive to 2-methyltetrahydrofuran in diesel engines. It was revealed [6,7] that not only as a pure fuel, but also as a blending component, DnBE allows for a strong decrease of exhaust emissions in comparison to conventional diesel fuels. Recently, *n*-octanol was applied as a neat fuel in diesel engines by Heuser et al. [8]. Almost NO_x and soot free combustion was observed over a wide range of engine loads.

While both biofuel candidates, DnBE and *n*-octanol, have demonstrated the ability to strongly reduce exhaust emissions in engine experiments [6–8], investigations are still required to explore their performance in terms of fuel efficiency. The well-known cetane number (CN) allows for the rough assessment of the fuel quality in diesel engines, before detailed numerical and experimental studies become available. The cetane number of fuels combines atomization, evaporation, mixture formation, and ignition properties into one global parameter. In general, it correlates strongly with the chemical ignition delay times of fuels, as is the case for DnBE. As shown in Ref. [4], DnBE ignites with very short induction times, and a high cetane number of 100 is reported [6]. However, the difference in the auto-ignition propensity of *n*-octanol and *n*-octane is relatively small compared to the difference in their cetane ratings [5]. While the ignition delay times of *n*-octanol are very similar to those of *n*-octane, cetane ratings of 39.1 and 63.8 are reported for *n*-octanol [9] and *n*-octane [10], respectively. The difference in their cetane numbers can thus be attributed only partly to the ignition delay times. In order to understand this phenomenon and to identify the crucial chemical and physical parameters, detailed numerical and experimental investigations are required.

The purpose of this study is to comprehensively investigate combustion of the biofuels *n*-octanol and DnBE in diesel engines. An important aspect here is not only to investigate the engine performance of these fuels separately, but also to investigate them together in order to assess the influence of molecular structure and functional groups on the engine combustion behavior. DnBE and *n*-octanol are investigated computationally and experimentally in a diesel engine, along with *n*-octane as a reference fuel. Studying *n*-octane helps to separate the effect of fuel oxygen content from other fuel properties. Its physical properties are quite similar to DnBE, while the ignitability of *n*-octane lies in between that of DnBE and *n*-octanol. The engine performance of these three fuels is compared with respect to their ignition behavior, heat release rates, and pollutant emissions. The effects of chemical and physical fuel properties, mixture formation, as well as scalar dissipation on engine operation are analyzed and discussed in detail.

Experiments of DnBE, *n*-octanol, and *n*-octane that have been performed in a single-cylinder diesel engine at four load points will

be presented. Pressure traces and heat release rates were measured along with unburned hydrocarbons, CO, and NO_x emissions in the engine experiments. To assess fuel structure effects and formation mechanisms of pollutant emissions in detail, the experiments are complemented with numerical simulations. Simulations were performed using the Representative Interactive Flamelet (RIF) model [11–13], which has been applied in many studies modeling compression ignition in internal combustion engines. The flamelet model can be derived from the governing equations [14] under the assumption that combustion is fast compared with the small-scale turbulent motions. The RIF model was derived particularly for describing unsteady ignition and combustion processes in compression ignition engines [12,13]. The model has been successfully applied in many applications [15–18] and it has recently been tested and validated using direct numerical simulation (DNS) data [19,20] showing very good accuracy for ignition and combustion for various different operating conditions. A general review of the model and its applications can be found in [21]. By the use of detailed chemical reaction mechanisms, the RIF model inherently accounts for low and high temperature auto-ignition, heat release, and pollutant formation [12,21–23]. Recently published chemical mechanisms for DnBE [4], *n*-octanol [5], and *n*-octane [24] are used to describe the combustion chemistry of the respective fuels.

The aim of the present paper is to understand and explain the effects of fuel properties on diesel engine combustion. Although the three fuels studied here are very similar in some respects, both the cetane numbers of the three fuels found in the literature and the experimental evidence presented here indicate that their behavior in diesel engines is very different. The reason could be physical properties, chemistry, or other differences. Therefore, numerical simulations, which are shown to reproduce the experimental evidence, are used in this study to investigate and explain the differences.

The paper is organized as follows: First, the molecular structures as well as the chemical and physical characteristics of the fuels are introduced. Afterwards, the combustion modeling approach is presented, followed by the description of the experimental setup and the engine operation conditions. In the results section, the engine simulations of the three fuels are compared to the experiments and with each other to reveal the fuel structure effect on combustion properties. This is complemented by detailed analyses of the differences in pollutant formation and heat release rates for the investigated fuels at various load points. Finally, the conclusions and major findings of this study are summarized.

2. Physical and chemical fuel characteristics

In this section, the physical properties and chemical kinetics of *n*-octane, *n*-octanol and DnBE are presented and discussed. First, their molecular structures are introduced and the physical and chemical characteristics are presented and discussed briefly. Subsequently, the ignition propensity of these fuels is studied in more detail in terms of chemical numerical modeling.

The molecular structures of *n*-octane, *n*-octanol, and DnBE are presented in Fig. 1. All three fuels consist of a straight chain with eight carbon atoms. While *n*-octane is not oxygenated, an O atom can be found at the end of the carbon chain in *n*-octanol and in the middle in DnBE. These alcohol and ether functional groups result in different ignition and combustion behavior of these fuels in comparison to alkanes. In general, the O atom has been found to reduce C–H bond dissociation energies (BDEs) at alpha carbon sites connected to an O atom and to increase BDEs at beta sites, as found in alcoholic fuels [25,26] and DnBE [4]. This leads to a quicker H abstraction at the alpha sites and could eventually accelerate auto-ignition, which has been demonstrated for the example of DnBE combustion [4]. For the case of alcohols, the presence of the hydroxyl moiety enhances H atom abstraction from the alpha carbon site as well, but it also

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