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Performance of lignin derived aromatic oxygenates in a heavy-duty diesel engine

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HIGHLIGHTS

- Two kinds of lambda variations of engine operation were presented.
- The effects of the molecular structures of aromatic oxygenates were discussed.
- The soot-NOx trade-off has been analyzed in details.
- The discussions on fuel consumption and engine efficiency were treated.

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ABSTRACT

The possibility to reduce dependence on fossil fuel resources has led to an increasing interest in the use of bio-fuels. This study builds on earlier work on (aromatic) cyclic oxygenates [1,2], but a far wider window of engine operation has been investigated in this paper. Two parametric variations of engine operation were performed and discussed: (1) non-EGR operation by means of varying the load via injection duration/quantity without EGR and (2) EGR operation by gradually increasing the level of EGR. The aromatic oxygenates in question are anisole, benzyl alcohol and 2-phenyl ethanol. The purpose of this work is to evaluate the feasibility of these lignin-derived bio-fuels in a compression ignition (CI) engine with a wide operation range and to assess the impact of the position of the functional oxygen group relative to the aromatic ring. For a better understanding of the combustion process, Heat Release Rates (HRR) have been compared and emissions of soot, NOx and unburnt products (HC, CO) have also been evaluated. The results demonstrate that both the soot-NOx trade-off and engine efficiency are improved for all oxygenates with respect to diesel. Moreover, the results indicate that EGR plays a very important role in further improving aforementioned tradeoff. With EGR, the improvement in the soot-NOx trade-off correlated to some extent with the position of the functional oxygen group to the ring, with better overall emission behavior observed as the oxygen group was farther removed (i.e. separated by carbon atoms) from the ring in the order anisole → benzyl alcohol → 2-phenyl ethanol. However, with respect to indicated efficiency, benzyl alcohol blend performed best in both non-EGR and EGR operation.

1. Introduction

Lignin, a biomass waste stream currently burnt in paper mills and cellulosic ethanol plants for process heat and electricity, has a unique poly-aromatic structure (Fig. 1). What is more, this second generation form of biomass is the only large-scale renewable feedstock for aromatics. Accordingly, if renewable aromatics are desired, it is inevitable that lignin no longer be burnt for low value process heat, but rather be depolymerized into useful (mono) aromatic base chemicals for the chemical industry. It is further foreseeable that in such a lignin-based refinery there will be a significant side stream of aromatics for fuel applications (Fig. 1). Against this background, it is worthwhile to study how such aromatic compounds will affect engine performance.

This study builds on earlier work on (aromatic) cyclic oxygenates. In [1,2], the soot-NOx trade-off and fuel efficiency of various aromatic oxygenates have been investigated on a modern DAF heavy-duty diesel engine. The aromatics in question, anisole, benzyl

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Abbreviations: BTDC, Before Top Dead Center; BD, Burn Duration = CA90-CA5; CA5, Time of 5% Cumulative Heat Release; CA10, Time of 10% Cumulative Heat Release; CA50, Time of 50% Cumulative Heat Release; CA90, Time of 90% Cumulative Heat Release; CN, Cetane Number; EGR, Exhaust Gas Recirculation; HHV, High Heating Value; HRR, Heat Release Rate; IMEP, Indicated Mean Effective Pressure; ID, Ignition Delay = CA10-SOI; ISFC, Indicated Specific Fuel Consumption; LHV, Lower Heating Value; MON, Motor Octane Number; RON, Research Octane Number; SOI, Start of Injection; TDC, Top Dead Center; η, efficiency; λ, Air-excess ratio.

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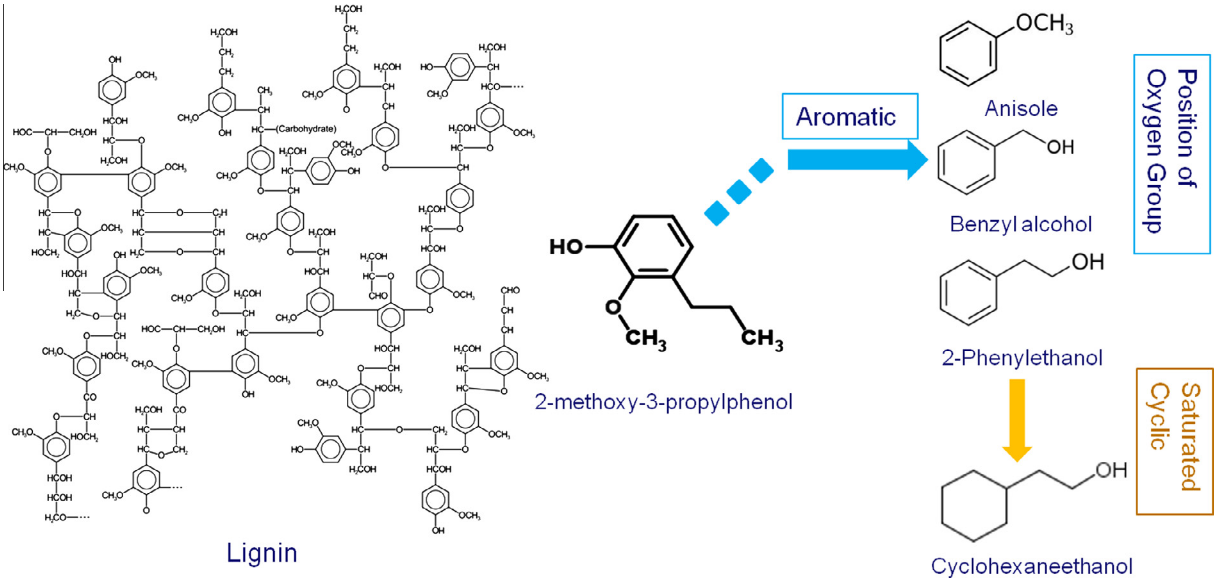

Fig. 1. Lignin and optional monomers for transport fuel applications.

alcohol and 2-phenyl ethanol, have similar heating values and Cetane Numbers, but differ in the type of functional oxygen group attached to the aromatic ring. Different functional groups were selected because the depolymerization of lignin will yield various types aromatic oxygenates. From the results [2] it becomes clear that both the soot-NOx trade-off and fuel economy are improved for all oxygenates in all investigated operation points. In general, the improvement in the soot-NOx trade-off correlated with the number of carbon atoms which separated the oxygen atom and the ring (e.g. 0 and 2 for anisole and 2-phenylethanol, respectively). Overall better soot-NOx trade-offs were observed for a greater number of carbon atoms separating aforementioned groups.

In the referenced earlier work, the number of operation points was quite limited, so this paper examines a far wider window of engine operation. Two parametric variations of engine operation will be presented for λ; one is non-EGR operation, by means of varying the load via injection duration/quantity and the other is EGR operation, by gradually increasing the level of Exhaust Gas Recirculation (EGR). The main purpose of this work is not only to evaluate the impact of EGR on overall engine performance, while using diesel as well as oxygenate blends, but also to investigate the effect of oxygenate molecular structures on the characteristics of CI engine running in a wider operation range. The discussion on fuel consumption and engine efficiency are also treated. Moreover, the soot-NOx trade-off will be analyzed in details by dividing the combustion conditions into three distinct regimes, which range from rich to lean mixtures.

2. Materials and methods

2.1. Fuels

As mentioned earlier, lignin has a poly-aromatic molecular structure. It therefore has to be depolymerized into useful monomeric aromatics as schematically illustrated in Fig. 1. This paper will not deal with the depolymerization method itself, but rather assume that such a method will eventually become available on a commercial scale to supply the chemical industry with highly desired renewable aromatic base chemicals.

The mono-aromatics can further be hydro-treated to form saturated cyclic oxygenates (e.g. cyclohexane ethanol). This study, however, will confine itself to the aromatic oxygenate in Table 1.

The three aromatic oxygenates in question are assumed to be of low toxicity for humans given that the US Food and Drug Administration (FDA Part 172, Subpart F) has approved their use as food additives for direct addition to food for human consumption, where they are typically used as flavorants (e.g. 2-phenyl-ethanol = rose). Relevant physical properties are presented in Table 1. From these can be inferred that boiling points of the neat oxygenates are on the low side of the diesel boiling range and that their densities are quite high. This study will not investigate the effects of density and boiling behavior on the emissions performance. It is assumed here that the chemical properties listed below (Table 2) are chiefly responsible for the difference in overall performance with respect to conventional diesel fuel. The methodology for the evaluation of the Lower Heating Value (LHV), Cetane Number (CN) and stoichiometric ratio can be found in Appendix.

2.2. Setup

The test engine, named CYCLOPS [5], is a test rig, designed and built at the Eindhoven University of Technology. It is based on a DAF XE 355 C heavy-duty truck engine. Specifications of this engine are presented in Table 3. Cylinders 4–6 operate under the stock engine control unit, and together with a water-cooled, eddy-current Schenck W450 dynamometer, they are only used to start the engine and control the rotational speed of the test cylinder, i.e. cylinder 1.

When data acquisition is idle, for instance during engine warm-up or in between measurements, only the three propelling cylinders are fired. Once warmed up and operating at the desired engine speed, combustion phenomena and emission formation can be studied in the test cylinder. Apart from the shared camshaft and crankshaft and the lubrication and coolant circuits, the test cylinder operates autonomously from the propelling cylinders. Fed by an Atlas Copco air compressor, the intake air pressure of the test cylinder can be boosted up to 5 bar. The fresh air mass flow is measured with a Micro Motion Coriolis mass flow meter. Non-firing cylinders 2 and 3 function as Exhaust Gas Recirculation (EGR) pumps (see Fig. 2, the schematic layout of the setup). Their purpose is to generate adequate EGR flow, even at elevated charge pressures.

Fueling of cylinder 1 is provided by a double-acting air-driven Resato HPU200-625-2 pump, which can deliver a fuel pressure up to 4200 bar. An accumulator is placed near (~0.2 m) the fuel