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# Comparison of emissions and performance between saturated cyclic oxygenates and aromatics in a heavy-duty diesel engine



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#### HIGHLIGHTS

• Study the impact of aromaticity of biofuels on emissions in a CI engine.

• 2-Phenyl ethanol is benchmarked against is saturated equivalent cyclohexaneethanol.

• Blends were prepared both at equal fuel oxygen and CN.

• Engine experiments were conducted by means of two lambda sweeps.

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#### ABSTRACT

Emissions and fuel economy are evaluated for two types of biofuels, namely 2-phenyl ethanol and cyclohexaneethanol. Both are derived from lignin, a form of lignocellulosic biomass. The former and latter oxygenates have an aromatic and aliphatic (i.e. saturated) ring structure, respectively. Two parametric engine sweeps were performed. First, non-EGR operation by means of varying the load via injection duration/quantity. Second, EGR operation by gradually increasing the level of EGR. The goal of this work is to evaluate the overall performance of these lignin-derived biofuels in a compression ignition (CI) engine over a wide range of operation conditions. More specifically, the research is focused on the effect of oxygenate aromaticity. The rationale behind this is that, starting from lignin, itself an aromatic molecule, it would require an expensive hydrogenation step to ultimately produce saturated ringed oxygenates like cyclohexaneethanol from the more lignin-like 2-phenyl ethanol. If there are no adverse effects of using the latter over the former, it makes no sense to consider further hydrogenation upgrading. The engine experiments have been conducted on a modified DAF heavy-duty diesel engine. The results demonstrate that further processing of aromatic oxygenates by means of hydro-treating to saturated rings is not only expensive, but also disadvantageous for the NOx-soot trade-off.

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#### 1. Introduction

In the search for alternative fuels, bio-derived fuels and their blends with diesel have been applied key interest. Bio-fuels are renewable fuels which are capable of replacing mineral based non-renewable fossil fuels. Mixing of bio-fuels with diesel has an influence on the combustion products and therefore on the soot and NOx concentrations within the exhaust gas.

It is known that the bio-fuels show different properties with respect to normal diesel. For instance, a lower cetane number (CN) leads to a longer ignition delay which results in a better premixing and brings about benefit from lower soot emissions. Furthermore, different studies have shown the positive influence of oxygen content in the fuel on the emission behavior [1–3]. Ramadhas et al. [4] claimed that, while using bio-fuels, the presence of oxygen in the structure of the bio-fuels increases the availability of reactive oxygen which will leads to an increase in combustion efficiency, thus improving oxidation resulting in reduction of soot, but an increase in NOx. Therefore, the amount of oxygen in the structure of the fuel molecule is critical in the views of both combustion and emissions [5,6].

Second-generation liquid bio-fuels are generally produced from lignocellulosic biomass, whose main advantage over first generation bio-fuels is that they are derived from non-edible feedstocks. 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). Lignin is the only large scale and renewable source for aromatics. Accordingly, it is inevitable that lignin bio-refineries will emerge in the not so distant future. In such a refinery, it is likely that not all aromatics can be used in the chemical industry, thereby creating a side stream of



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Nomenclature			
BTDC BD CA5 CA10 CA50 CA90 CN EGR HHV HRR IMEP	before top dead center burn duration = CA90–CA5 time of 5% cumulative heat release time of 10% cumulative heat release time of 50% cumulative heat release time of 90% cumulative heat release cetane number exhaust gas recirculation high heating value heat release rate indicated mean effective pressure	ISFC LHV MON PM RON SOI TDC $\eta$ $\lambda$	indicated specific fuel consumption lower heating value motor octane number particulate matter research octane number start of injection top dead center efficiency air-excess ratio
ID	ignition delay = CA10-SOI		

(oxygenated) aromatics for the transport fuel market. This vision underlines the importance to investigate the compatibility and performance of oxygenated aromatics in diesel engines.

This paper builds on earlier engine work performed with cyclic oxygenates. In [7], the authors compare aromatic against saturated cyclic oxygenates and report comparable emission behavior between the two. From a production point of view, starting from lignin – itself a polymer of aromatic oxygenates – it would be far more economical to focus on aromatic end-products. Saturated compounds, conversely, would require large amounts of expensive hydrogen to produce. Accordingly, this line of research will focus primarily on aromatic oxygenates. This paper aims to add additional insight into the case for aromatics oxygenates as renewable diesel components by investigating an extended measurement strategy which covers wider engine operation range. Fuels will be evaluated first with constant fuel oxygen content. Second, the fuels will be compared at equal CN.

On the other hand, improving the NOx-Soot trade-off is one of the most important goals in diesel engine research and it is well-known that this trade-off hinges heavily on fuel molecular structure [8]. Moreover, the use of exhaust gas recirculation (EGR) to reduce NO<sub>x</sub> has been investigated extensively before [9–11]. Consequently, investigation of the NOx-soot trade-off for various

fuels, both with and without EGR, is one of the focuses in this study.

In the referenced earlier work [7], the number of work 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 lambda ( $\lambda$ ); 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 EGR. The main purpose of this work is not only to evaluate the impact of EGR on overall engine performance, but also to investigate the impact of aromaticity in lignin-based bio-fuels. This evaluation will be made first at equal fuel oxygen content and second with equal CN.

#### 2. Materials and methods

#### 2.1. Fuels

As a poly-aromatic molecular structure material, lignin has to be depolymerized into practical, ideally monomer (i.e. single ring) aromatics. The depolymerization process itself is out of the scope of this paper, it assumes that such a process, most likely

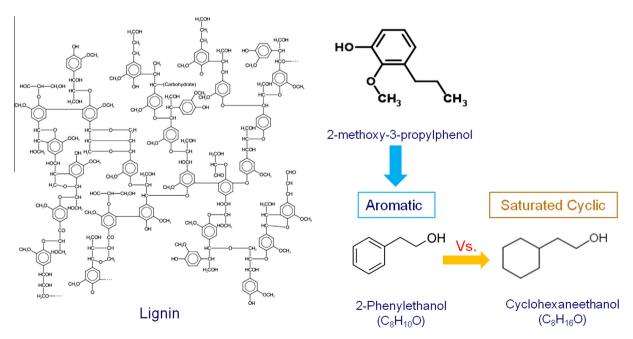


Fig. 1. Lignin and possible monomers for transport fuel applications.

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