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# Combustion analysis of methane-hydrogen port injection combined with $OME_n/Diesel$ spray injection in an RCCI engine

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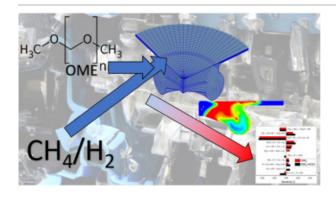
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#### Abstract

<u>Compressed Natural Gas</u> (CNG) is recognized as an environmentally friendly alternative vehicle fuel, but it has a low flame speed. Combining hydrogen with CNG to create 'hydrogen compressed natural gas' (HCNG) allows for faster and leaner combustion. Additionally,  $OME_{2-4}$  with varying <u>cetane numbers</u>, from 63 for  $OME_2$  to 90 for  $OME_4$ , serves as a highly reactive fuel suitable for use in a dual fuel strategy known as RCCI (reactivity-controlled compression ignition). This project investigates the impact of adding  $OME_{2-4}$  to HCNG, focusing on pressure, temperature, and emissions. Results indicate that lengthening the OME chain advances the <u>peak heat release rate</u> but delays the second combustion phase. In <u>diesel + HCNG</u>, the first-phase combustion is 2 °CA shorter than  $OME_2 + HCNG$ , resulting in a 6.5% higher peak pressure than  $OME_2 + HCNG$  and a 20% increase over basic diesel. Lengthening the OME chain from  $OME_2$  to  $OME_4$  raises the peak pressure by about 6.2%. The addition of gaseous fuels, especially hydrogen, increases peak

temperature by 16%. **OME**<sub>4</sub> + **HCNG** has a similar peak temperature to **OME**<sub>3</sub> + **HCNG**, while **OME**<sub>2</sub> + **HCNG** is about 1.5% lower than **OME**<sub>4</sub> + **HCNG**.

#### Graphical abstract



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## Introduction

In today's modern world, increasing demand for transportation due to new technologies is rapidly raising energy consumption, mainly from fossil fuels like petroleum [1]. Diesel engines are crucial in ground transportation but face emission challenges [2]. Recent research has shown that it's possible to reduce both soot and NO<sub>x</sub> emissions simultaneously through methods like fuel injection under pressure, supercharging compression, and fuel additives for PM (particulate matter) reduction, along with exhaust gas recirculation (EGR) for NO<sub>x</sub> reduction [[3], [4], [5]]. Population growth and improved living standards are driving up fossil fuel consumption, leading to a 36% increase in total energy consumption over the last 15 years [6,7]. This rising energy demand necessitates increased fuel production, depleting fossil fuel reserves at a faster rate [8].

Depleting petroleum reserves and environmental concerns have spurred the search for alternative fuels like compressed natural gas (CNG), hydrogen, liquefied petroleum gas (LPG), and carbon-neutral synthetic fuels [1]. While hydrogen faces obstacles like storage and distribution, hydrogen and CNG blends (HCNG) offer a more viable automotive fuel option without major engine or infrastructure changes [9]. It enables leaner burning, extending the lean operating limit, reducing hydrocarbons and CO [5,6]. HCNG offers torque and thermal efficiency comparable to CNG, with potential for higher thermal efficiency by compromising some NO<sub>x</sub> gains. It lowers greenhouse gas emissions like CO<sub>2</sub> due to increased H/C ratio [10]. HCNG's high hydrogen flame speed optimizes combustion, enhancing the heating value and engine performance [7,8].

Synthetic fuels like OME (oxymethylene ethers) are produced from renewable sources and can reduce  $CO_2$  emissions [11,12]. Hydrogen for internal combustion engines is also explored, with polyoxymethylene dimethyl ethers (**OME**<sub>n</sub>), the molecular formula of **CH**<sub>3</sub>**O**(**CH**<sub>2</sub>**O**)<sub>n</sub>**CH**<sub>3</sub> (Fig. 1), showing promise in reducing engine emissions, especially soot [13,14]. These synthetic fuels, lacking C–C bonds, significantly reduce soot formation, as soot formation involves two mechanisms: particle formation and oxidation [2,15].

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OME/air mixtures have additional fuel-oxygen bonds, making them leaner and reducing soot formation due to increased OH radicals [16,17]. **OME**<sub>n</sub> fuels offer a significant reduction in soot emissions and avoid the trade-off between soot and nitrogen oxides (NO<sub>x</sub>). They can be produced from renewable sources through various methods, including power-to-liquid (PtL) and biomass processes [18]. These fuels are fully compatible with conventional hydrocarbon fuels and have high cetane numbers (e.g., 63 for OME<sub>2</sub> up to 90 for OME<sub>4</sub>), which improves diesel fuel ignition behavior [19,20].

Reactivity controlled compression ignition (RCCI) is a dual fuel strategy that uses fuels with different reactivity in order to improve the combustion process and reduce emissions from a diesel engine. Combustion characteristics of the engine under RCCI mode are controlled by varying the quantity and injection timings of the dual-fuel charge (high and low reactivity fuels). In dual fuel and RCCI engines [21,22], adding hydrogen boosts ignition and peak pressure [23,24]. Injection strategy is crucial for combustion control. With hydrogen/methane as the low reactivity fuel, NO increases while CO decreases [25,26]. RCCI engines using diesel and natural gas can cut fuel consumption by up to 60% [27]. Combustion with HCNG-air and OME works in RCCI mode [28,29]. Hydrogen mainly affects early combustion stages without excessive noise or knock [30,31].

Polyoxymethylene dimethyl ethers ( $OME_n$ ) are polyether compounds with a structure similar to methylal, formed by inserting oxymethylene groups ( $-CH_2O-$ ) into the methylal molecule [32,33].  $OME_n$  possess unique physicochemical properties including low toxicity, excellent volatility, low condensation point, high permeability, good solubilization capacity, and compatibility with organic compounds and water [34]. Their C-O and C-C bond lengths (0.143 nm and 0.154 nm, respectively) result in higher density compared to n-alkanes, with density inversely related to temperature and directly related to chain length [34]. For more details, refer to Table 1.

In the realm of combustion dynamics within RCCI engines, a conspicuous gap in comprehensive research concerning the cascading effects of **OME**<sub>n</sub> fuels has come to light through an exhaustive review of existing literature. Our current investigation not only bridges this void but also advances our comprehension by providing a pertinent comparison between OME and conventional high reactivity diesel fuels within the context of RCCI combustion. Our study primarily focuses on elucidating the impacts of **OME**<sub>2-4</sub> and diesel fuels in conjunction with hydrogen and methane (HCNG), known for its lower reactivity, under demanding operating conditions of 1250rpm at full load. The goal is to comprehensively evaluate engine behavior, benchmarked against conventional diesel combustion. To achieve this, we employ advanced software tools. Chemkin software aids in 0-1D analysis, enabling an exploration of key parameters like laminar flame speed, reaction pathways, and sensitivity across various fuel configurations. Furthermore, we leverage AVL Fire software, along with its workflow manager module, to facilitate intricate 2-3D simulations.

# Section snippets

# Materials and methods

In the methodology section of the research, a clear demarcation between the experimental and simulation components are implemented to ensure transparency and comprehensibility in the investigative process....

## Results and discussion

This research concerns the modification of a conventional diesel engine into an RCCI engine that uses HCNG (composed of 60%  $CH_4$  and 40%  $H_2$ ) as a low reactivity fuel, and  $OME_{(2-4)}$  and diesel as high reactivity fuels (HCNG constitutes 0.5% of the incoming air mass fraction, meaning that 0.5% of the air entering the chamber is HCNG). To ensure a fair comparison, the volume of injected fuel for the base engine (diesel) remains constant across all cases, and the injected mass varies based on the...

# Conclusion and future perspectives

This study investigates the combustion of an HCNG blend, along with **OME**<sub>n</sub> and diesel, in an RCCI engine, where HCNG serves as the low reactivity fuel, and **OME**<sub>n</sub> and diesel serve as the high reactivity fuels. The results reveal that as the OME chain length increases, the combustion duration in the first phase (**MFB**<sub>10-50</sub>) decreases due to lower volatility and a higher cetane number. However, lengthening the OME chain increases the duration of the second combustion phase (**MFB**<sub>50-90</sub>). The shorter...

# Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper....

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