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Full Length Article

Homogeneous charge compression ignition (HCCI) combustion of polyoxymethylene dimethyl ethers (PODE)

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HIGHLIGHTS

- Characteristics of PODE HCCI combustion were investigated for the first time.
- PODE HCCI exhibits two-stage ignition with strong low temperature heat release.
- Detailed combustion and emission data under various Φ_m and EGR conditions were studied.
- PODE lean HCCI combustion produces ultra-low NOx and soot emissions.
- PODE lean HCCI combustion forms reactive hot atmosphere.

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ABSTRACT

Polyoxymethylene dimethyl ethers (PODE) are a promising alternative fuel for diesel engines. PODE have high volatility, high ignitability and high oxygen content, and is thus also an ideal additive fuel for blend and dual-fuel combustion due to its low-temperature chemistry. In this work, the characteristics of PODE homogenous charge compression ignition (HCCI) combustion are investigated for the first time. The effects of charge mass equivalence ratio (Φ_m) and exhaust gas recirculation (EGR) on PODE HCCI are studied. The results indicate that PODE HCCI exhibits two-stage ignition with a strong low temperature heat release (LTHR) before the high temperature heat release (HTHR). HTHR switches from one-stage to two-stage with an increase of Φ_m due to rapid CO oxidation. At a specific EGR rate, with an increase of Φ_m, the end-of-compression charge temperature decreases, the ignition timing of LTHR delays. With an increase of Φ_m, the ignition timing of the HTHR advances at the EGR lower than 42%, but it delays at the EGR of 52% in general. For a specific Φ_m, with an increase of EGR, the end-of-compression charge temperature decreases, the ignition timing of both LTHR and HTHR delays, and the combustion duration of the HTHR increases. CO emissions decrease with an increase of Φ_m and a decrease of EGR. Φ_m and EGR have only a slight effect on HC emissions. This work also provides fundamental data of PODE combustion characteristics for the future development of PODE reaction mechanisms.

1. Introduction

Among various oxygenated fuels, alcohols, esters and ethers are the three major categories that can be used as engine fuels (Fig. 1). Alcohols have a high octane number, and are usually used as gasoline substitutes for a spark ignition (SI) combustion. Long-chain esters have a high cetane number, and are usually used as diesel substitutes. However, the soot reduction potential of esters is not ideal because their oxygen content is only 10% due to the existence of only one ester group (—COOR). Whereas, ethers have a high cetane number and a high oxygen content because more than

Abbreviations: PODE, polyoxymethylene dimethyl ethers; Φ_m, charge mass equivalence ratio; LTHR, low temperature heat release; AC, absorption coefficient; MPRR, maximum pressure rise rate; COV, coefficient of variation; TS HTHR, two-stage high temperature heat release; HC, hydrocarbon; RoHR, rate of heat release; HCCI, homogenous charge compression ignition; EGR, exhaust gas recirculation; HTHR, high temperature heat release; Φ, equivalence ratio; IMEP, indicated mean effective pressure; OS HTHR, one-stage high temperature heat release; SOI, start of ignition; CO, carbon monoxide; DICI, direct injection compression ignition.

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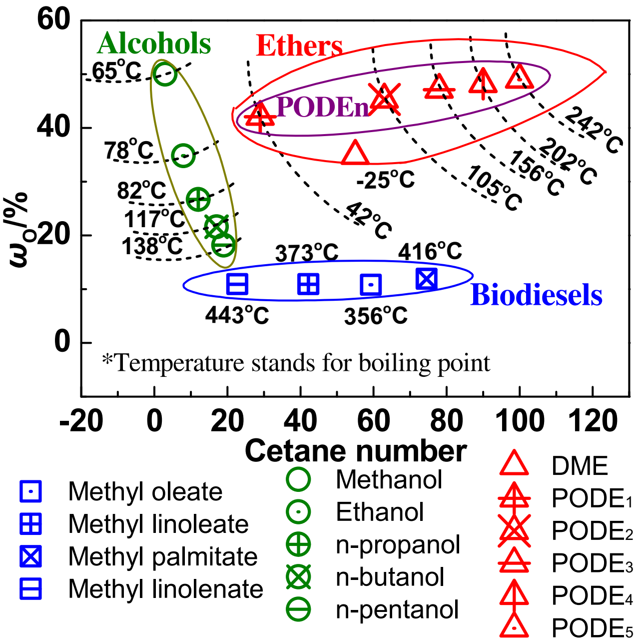

Fig. 1. Oxygen content and cetane number of oxygenates (cetane number date are cited from Ref. [2]).

one —CH_2O— unit can exist in the short-chain ether molecule. The molecule structure also excludes C—C bonds, impling that ethers are more efficient in reducing soot emissions than other oxygenates [1]. Therefore, ethers are best among the three categories for compression ignition (CI) combustion.

Polyoxymethylene dimethyl ether (PODE) are a promising ether fuel for diesel engines because it contains nearly 50% oxygen and has a high cetane number. PODE can be synthesized from methanol. Low-cost commercial production of PODE has recently been realized in China [3,4]. In 2012, Tsinghua University developed an industrial technique for producing PODE with the capacity of 10 kton/year in China, and the cost of production is close to that of diesel. Fig. 2 shows the technological process of PODE synthesis. Methylal is synthesized from formaldehyde solution and methanol over heterogeneous acid catalyst. Methylal then reacts with paraformaldehyde forming PODE components. The desired PODE components to be blended with diesel are $PODE_{3-5}$ and the ratio of the three components can be changed by adjusting reaction conditions. Unconverted methylal and undesired short-chain $PODE_2$ compound are fed back to the reactor. Undesired long-chain PODEn (n > 5) compounds are recycled as solid fuels. Engine combustion studies using PODE as a diesel fuel additive have been conducted. Diesel blends with 10–20% PODE by volume [5] in a direct injection diesel engine can significant reduce carbon monoxide (CO), hydrocarbon (HC) and particulate matter (PM) emissions and slightly increase thermal efficiency. With the application of EGR, NOx emissions are also very low. Further studies have reported that PODE can break the soot-NOx trade-off relationship in both diesel/PODE blends for direct injection compression ignition (DICI) [6,7] and PODE-gasoline [8] dual-fuel combustion. These combustion paths for low emissions and high efficiency are related to the fuel stratification [9] and active hot atmosphere [10,11] formed by PODE low-temperature reactions before diesel [6,7] or gasoline [8] ignition. In these combustion methods, the main fuels, such as gasoline and diesel are usually present at concentrations higher than 70%. PODE premixed mixture auto-ignition usually occurs (before TDC). Therefore, homogeneous charge compression ignition (HCCI) of PODE under lean mixture conditions needs to be investigated to better understand the above combustion paths for low emissions and high efficiency.

The objective of this work is to investigate the combustion process of PODE HCCI combustion. The effects of fuel equivalence ratio and EGR rate on both the low temperature heat release (LTHR) and the high temperature heat release (HTHR) are studied. The heat release and emission data are also provided in the supplementary material, and are valuable for chemical kinetic studies of PODE combustion mechanisms.

2. Fuel selection and experimental setup

2.1. Selection of test fuel

Fig. 3 shows the cetane number and boiling point of PODEn (n stands for the polymerization degree), gasoline and diesel, and properties of $PODE_n$ are provided in Table 1. Fuels with LTHR require lower intake temperatures than fuels without LTHR, so using fuels with LTHR can simplify the structure of intake systems. In Ref. [12], Bunting et al. found that at naturally aspirated conditions no LTHR was detected for fuels with CN < 35. Therefore, the ideal cetane number for HCCI should be higher than 35. For $PODE_n$ ($CH_3O(CH_2O)_nCH_3$), the cetane number and boiling point both increase with an increase of polymerization degree (n). $PODE_2$ and $PODE_3$ lie in the ideal region for HCCI. However, $PODE_2$ does not fulfill security criteria because of its low flash point (−28 °C) [13]. Thus, $PODE_3$ is the optimal candidate for the HCCI combustion

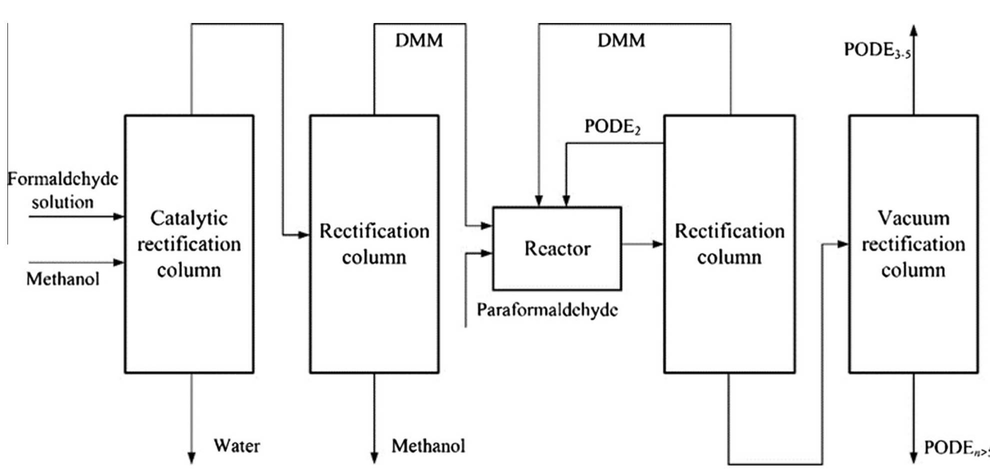

Fig. 2. The technological process of PODE synthesis [5].