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A theoretical investigation of the effects of the low-temperature reforming products on the combustion of *n*-heptane in an HCCI engine and a constant volume vessel

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HIGHLIGHTS

- New combustion mode in the engines, flexible cylinder engine, is conceived.
- The new concept is comprehensively demonstrated using *n*-heptane as the fuel.
- The new strategy may reduce the ignition delay time of the fuel.
- The reformed fuel may alter the combustion reaction pathways in the cylinder.

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ABSTRACT

A new concept of the flexible cylinder engine for the combustion in the engine cylinders is developed to optimize the combustion process, according to the practical working conditions. By the new concept, the fuel is reformed in the flexible cylinder, mixed with the same fresh fuel, and then introduced into the normal cylinders to finish the normal combustion process. The reformed fuel may alter the combustion reaction pathways of the fresh fuel and hence may improve the combustion in the engine cylinders potentially. In this work, the effects of the reformed fuel on the combustion of the fresh fuel were investigated by using *n*-heptane as the model fuel to demonstrate this new concept theoretically. It was found that the reformed fuel may decrease the ignition delay time of the fresh fuel by about 6 TDCA (top dead crank angle) at a typical engine condition. Among the reformed species, ketohydroperoxides and hydrogen peroxide are the key species to decrease the ignition delay time besides the radicals. The reformed fuel may increase the laminar flame speed of the fresh fuel, with H_2 and CO being the key species. Finally, the reformed fuel may also decrease the harmful emissions, such as the unburned hydrocarbons, including acetylene, ethylene, propyne, propylene, 1,3-butadiene, and the partially oxidized species, including formaldehyde, ketone, acetaldehyde, etc. These simulation results indicate that the new concept of the flexible cylinder engine is a potential clean combustion strategy for the engines.

1. Introduction

The energy crises and the environment issues related to the use of the fossil fuels in the engines brought increasing challenges to the world [1–3]. Researchers have proposed many strategies [4–14] to improve the engine efficiency and to reduce the emissions to meet the increasingly stringent emission regulations, such as the homogeneous charge compression ignition (HCCI), the stratified charge compression ignition (SCCI), and the reactivity-controlled compression ignition (RCCI), etc. Basically, all of these strategies altered the combustion process to meet the regulations by optimizing the initial engine operation conditions and/or the fuel properties. In recent years, new strategies such as catalytic reforming combustion [15–18] and plasma reforming combustion [19], etc. were also investigated to optimize the combustion process in the engine cylinders. Yao et al. [20,21] catalytically reformed methanol using palladium as the catalyzer in a spark ignition engine and reported that the NO_x was decreased by 90% and CO by 50%. The researchers of the Southwest Research Institute [22,23] proposed the dedicated exhaust gas recirculation (D-EGR) theory to improve the efficiency and the emissions of the engine. According to the D-EGR theory, gasoline was partially catalyzed into small molecules (H_2 and CO, etc.) in a dedicated cylinder

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and was then introduced into the other cylinders fueled with fresh gasoline. The average thermal efficiency was increased by 12–15%. Researchers have also investigated the effects of the additions of different species into the fuels on the performances of the fuels in the engines experimentally and theoretically. Tanaka et al. [24] studied the effects of 2-ethylhexylnitrate and di-*tertiary*-butylperoxide additions into paraffins, cyclic paraffins, olefins, cyclic olefins, and an aromatic hydrocarbon, etc. on the combustions of these fuels. It was found that the additives resulted in reduced ignition delay times without affecting the burning rates for HCCI combustion. Lü et al. [25] experimentally investigated the effects of some combustion inhibitors (methanol, ethanol, *iso*-propanol, and methyl *tert*-butyl ether) on the combustion of *n*-heptane by port injection of them in an HCCI engine. The results indicated that ethanol was the most effective combustion inhibitor in expanding the operating range, improving the emissions and the thermal efficiency. Hammond et al. [26] investigated the effect of hydrogen peroxide (H_2O_2) addition on the combustion of CH_4 in an HCCI engine numerically. It was found that the addition of H_2O_2 can be used to control the combustion phase while maintaining the low emissions and the peak in-cylinder pressures. Manias et al. [27] simulated the effects of CH_2O and H_2O_2 additions into CH_4/air mixtures on the ignition delay times and reported that 1% of these species in the mixtures could decrease the ignition delay time considerably. These works indicated that the additions of certain species may improve the combustions in the engines. However, an engine should be operated in a broad range depending on the practical conditions, and hence the additives should be introduced at different ratios flexibly. The dual fuel strategy [28–30] may meet this requirement. But this strategy introduces an extra tank for the additive, even an extra catalyzing device in the catalyze-reforming mode. These strategies will inevitably increase the burden of the vehicle. Based on the previous strategies, a new concept, flexible cylinder engine (FCE), is developed to provide with the additives reformed from a single fuel and hence no extra tank will be needed. Fig. 1 shows the schematic diagram of FCE. The engine mainly consists of a flexible cylinder and two or three normal cylinders. In the full-load condition, the flexible cylinder will operate at the same parameters with those of the normal cylinders, to ensure the required output power and torque. While in the part-load condition, the flexible cylinder may work as the reforming cylinder to provide with the suitable additives reformed from the fuel for the normal cylinders. The components of the reformed fuel can be flexibly controlled by a separate electric control unit and hence with different reactivities. The reformed fuel will then be mixed with the fresh fuel and injected into the normal cylinders to work as a normal fuel. The advantages of this concept are obvious. Firstly, the flexible cylinder can flexibly reform the fuel into the suitable additives to improve the combustion of the fuel. Secondly, the strategy avoids the installment of an extra additive tank and even a catalyzing device. Lastly, the flexible cylinder can be flexibly operated as a normal cylinder in the full-load condition and thus expand the operating range.

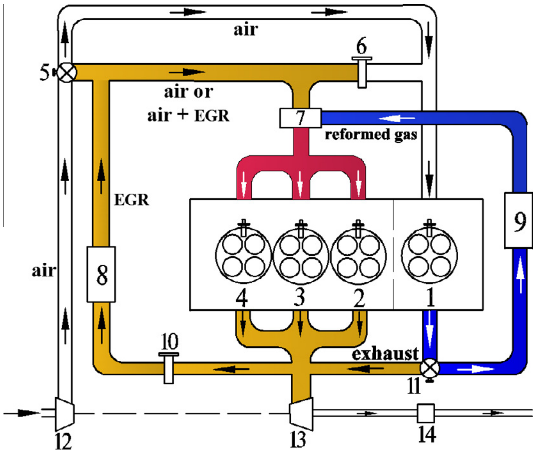

Fig. 1. Schematic diagram of the new concept of flexible cylinder engine. (1, Flexible cylinder; 2, 3, 4, Normal cylinder; 5, 11, Electric valve; 6, 10, Valve; 7, Premixing chamber; 8, 9, Cooler; 12, Compressor; 13, Turbine; 14, After-treatment device.)

FCE is different from D-EGR. D-EGR partially oxidizes the fuel with certain catalyst to increase the mass fraction of CO and H_2 and hence to improve the combustion, while FCE reforms the fuel to multiple species, including the typical low temperature combustion species of ketohydroperoxide, H_2O_2, CH_2O, H_2, and CO, by the low-temperature reformation to improve the ignition delay time, the laminar flame speed, and the emission of the fuel. D-EGR is applied in the spark-ignition gasoline engine with upgraded spark plugs, with gasoline as the fuel, while FCE aims at the HCCI diesel engine, with both gasoline and diesel being suitable as the fuel. The dedicated cylinder in the D-EGR engine is specially designed only to reform the fuel, while the flexible cylinder in the FCE engine may switches between a normal cylinder and the reforming cylinder flexibly, depending on the operation condition.

FCE is also different from other strategies, such as HCCI, SCCI, and RCCI, etc. As described in the previous texts, under the FCE mode, part of the fuel is reformed at low-temperature in the flexible cylinder and then mixed with the fresh fuel in the premixing chamber before being introduced into the normal cylinders together to improve the combustion flexibly according to the working conditions, while under the HCCI mode, all of the fuel is mixed with the air in the intake port to be ignited homogeneously in the cylinder. Under the SCCI mode, a larger proportion of the fuel is injected in the intake port and introduced into the cylinder. A small proportion of the fuel is then injected in the cylinder to form a layered mixture with different concentration zones. Under the RCCI mode, a fuel of low-reactivity is mixed with the air and recirculated gas in the intake port and introduced into the cylinder. Another fuel of high reactivity is then injected into the cylinder to control the in-cylinder fuel reactivity and hence to optimize the combustion phasing, duration, and magnitude. The FCE mode is different from the above combustion modes with its different spray strategy and its rationale. The FCE mode alters the composition of the original fuel in the normal cylinders and hence alters the reaction pathways of the fuel.

In this paper, *n*-heptane was used as the model fuel to theoretically demonstrate the new concept of FCE. *n*-Heptane is a vital component in both the surrogate fuels for gasoline and diesel and has a typical and fully-developed low temperature combustion process. To clarify the concept of FCE, only *n*-heptane was investigated in this work. The key low-temperature reformed products of *n*-heptane were mixed with *n*-heptane and injected in the normal cylinders as the starting fuel. The effects of these reformed additives on the combustion of *n*-heptane were investigated, including the ignition delay time, the laminar flame speed, and the formation of some key emissions. Reaction pathways analyses were also performed to clarify the formation of these species.

2. Models

A typical operation condition was selected to simulate the combustion in an HCCI engine with the SENKIN code of the CHEMKIN2.0 package [31]. The operation conditions of the flexible cylinder and the normal cylinders are shown in Table 1. The equivalence ratio (ϕ) in the normal cylinder was maintained at 0.6, while