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The impact of low temperature reforming (LTR) products of fuel-rich n-heptane on compression ignition engine combustion

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ABSTRACT

In order to achieve high-efficiency and clean combustion in compression ignition engines, combustion must be controlled reasonably. A great variety of species with various reactivity could be produced through low temperature oxidation of fuels, which offered possible solutions for controlling the total fuel reactivity flexibly in engines. In experiments, a set of LTR system was established on an optical compression ignition engine to investigate the impact of LTR products on combustion characteristics, and the planar laser-induced fluorescence of hydroxyl (OH-PLIF) measurements were conducted to illustrate the flame development. N-heptane was chosen as the feedstock fuel. In kinetic calculations, a FLOW REACTOR model was used to predict the components of LTR products, and an HCCI model was used to evaluate the reactivity of each LTR product. The reactor model analysis and GC–MS measurements indicate that n-heptane does not take oxidation reaction at low reformer temperature of 473 K. When the reformer temperature rises up to 523 K, LTR products mainly include hydrogen, carbon monoxide, olefins, aldehydes, alkanes, alkynes, alcohols and C_7 cyclic ethers through the prediction of the kinetic model. According to the experimental engine analysis, the ignition timing is retarded significantly and the heat release rate is slowed down due to the reactivity variety of in-cylinder mixture via LTR. The OH-PLIF images show that in addition to delaying the ignition timing and reducing the combustion rate, LTR also contributes to the improvement of in-cylinder combustion uniformity. The natural flame luminosity result indicates that less soot emission is formed in the combustion process by LTR. The reactivity evaluation using the kinetic modeling approach suggests that the ability of acetylene in improving reactivity is extremely strong, but the ability drops with the increasing mole fraction of acetylene. Though hydrogen, carbon monoxide, ethylene, propene and methane are present in large concentrations, they act to have little effect on mixture reactivity. However, most of the LTR products exhibit decreased mixture reactivity, which should cause a delay of the ignition in the experiment. The impacts of LTR products on ignition are influenced not only by the chemical structure, but also by the concentration in the mixture. It is inferred that the LTR products can control the ignition flexibly in compression ignition engines by changing reforming conditions.

1. Introduction

Energy shortage and environmental pollution are two major challenges in the development of internal combustion engines. Advanced combustion technology is the key to meet the stringent emission regulations and achieve high engine thermal efficiency. Therefore, researchers have put forward different new combustion modes, such as homogeneous charge compression ignition (HCCI) [1,2], premixed charge compression ignition (PCCI) [3,4], low temperature combustion (LTC) [5], reactivity controlled compression ignition (RCCI) [6,7] and gasoline compression ignition (GCI) [8], etc. In fact, these combustion modes are essentially achieved by changing combustion chemical reaction pathways to avoid the formation of pollutant and achieve higher efficiency, compared with the traditional combustion process. In recent decades, researchers have proposed concepts of fuel reforming to further optimize the combustion process in engines. Tsolakis et al. [9,10] investigated diesel reforming using a laboratory reforming mini reactor incorporated in the exhaust system of a diesel engine. Up to 16% (volume fraction) hydrogen in the reforming gas was achieved at a reactor inlet temperature of 290 °C. The results showed that the exhaust gas assisted diesel fuel reforming could reduce NO_X and smoke emissions in diesel engines. Later, they applied the reformed exhaust gas recirculation (REGR) technique [11,12] to PCCI combustion by using diesel and biodiesel. The technique involved the injection of hydrocarbon fuel into a catalytic reformer which was fitted into the EGR system. They found that REGR resulted in the higher premixed combustion rate and the

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reduction of the diffusion combustion phase in both cases. Shudo et al. [13,14] proposed a new concept HCCI engine system fueled with dimethyl ether (DME) with a high cetane number and methanol-reformed gas (MRG) that consisted of hydrogen and carbon monoxide with high anti-knock properties. In the system, both DME and MRG were produced from methanol by onboard reformers utilizing the engine exhaust heat. The results showed that a high overall thermal efficiency was achieved and the HCCI load could be expanded by adjusting the fraction of the two fuels. Barrett et al. [15,16] proposed the concept of dedicated EGR (D-EGR), which combined emission control technology and fuel reforming strategy together. In D-EGR, gasoline was catalytically reformed into small molecules (hydrogen and carbon monoxide, etc.) in a dedicated cylinder exhausting directly to the intake manifold. And then the reforming gas was introduced into the remaining cylinders to burn with fresh gasoline. D-EGR resulted in large gains in fuel efficiency over the baseline and significant exhaust emission reduction. Zhu et al. [17] implemented the thermochemical fuel reforming (TFR) concept in a spark ignition natural gas engine. Methane, hydrogen and carbon monoxide as the major reforming products of TFR cylinder over a range of rich equivalence ratios, were introduced into the other working cylinders. According to the experimental analysis, TFR was effective in simultaneously improving brake specific fuel consumption and reducing emissions.

As mentioned above, fuel reforming exhibits obvious advantages in improving emissions, combustion characteristics, thermal efficiency and fuel economy. However, applications of these fuel reforming concepts basically require an active and stable catalyst favoring a good conversion of feedstock fuel in a wide domain of temperatures. Furthermore, the selection of appropriate catalyst is complicated [18,19], and the catalyst in a reformer is easily poisoned by the sulfur content in engine fuels [17]. Moreover, it is only the hydrogen-enriched gas steam produced by fuel reforming that has beneficial effects on engine performances. In fact, in order to operate the engine in a broad range of speeds and loads, combustion must be controlled reasonably. Hence, the reformate reactivity that can be flexibly controlled is demanded.

Low temperature oxidation (500–800 K, typically in or below the negative temperature coefficient regime) of hydrocarbons could produce a great variety of species with various reactivity and the species concentration varied with initial conditions, which offered possible solutions for controlling the total fuel reactivity flexibly in engines. Low temperature oxidation of hydrocarbons is important in developing HCCI and traditional diesel engines. Then as an essential component of primary reference fuels for gasoline and a surrogate for large n-alkanes in diesel fuels, low temperature oxidation of n-heptane has been studied experimentally and numerically in jet-stirred reactors [20,21], flow reactors [22,23] and rapid compression machines [24,25]. These studies investigated low temperature speciation or improved the existing chemical kinetic model on the basis of experimental results. Various low temperature oxidation products of n-heptane in these investigations comprised carbon oxide, olefins, aldehydes, alkanes, alkynes, alcohols, cyclic ethers, etc. However, there is a lack of research on the impact of the products on the engine combustion.

In this work, the effect of LTR products of fuel-rich n-heptane on the engine combustion was explored by establishing a set of LTR system for the engine. Firstly, the LTR products from the reformer were analyzed through the predictions of the Lawrence Livermore National Lab (LLNL) detailed n-heptane reaction mechanism. Then the LTR products were introduced into the cylinder to conduct an experimental investigation. Most studies about fuel reforming were focused on results of improving engine performance and emissions, and insufficient attention was given to the relevant combustion process. Hence in the present work, in-cylinder flame development was investigated to promote a better understanding of the combustion phenomena by taking OH-PLIF images. Then to perform causal analysis of ignition timing variation due to LTR, the reactivity of each LTR product was evaluated by the kinetic model. Finally, an in-depth impact mechanism of LTR on engine combustion would be revealed, which will be an important direction in the application of LTR on engines.

Table 1
Optical engine specifications.

Parameter	Value
Number of valves	2
Bore	92 mm
Stroke	100 mm
Compression ratio	11:1
Number of holes	6
Hole diameter	0.15 mm
Spray angle	150°

2. Experimental setup

Experiments were carried out on an optical engine which was modified from a naturally aspirated four-cylinder diesel engine with two valves and an overhead camshaft. The optical engine specifications are presented in Table 1. The compression ratio is 11:1 to meet the optical design requirements. The schematic diagram of LTR system for the engine is shown in Fig. 1. It mainly consists of optical engine, inlet heating device, syringe pump (LONGER, LSP01-2A), air compressor (FENGBAO, FB-3617, China), gas flow meter (ALICAT, MC-5SLPM-D/5M, China), fuel evaporation mixer and low temperature reformer. Firstly, the air stream in the evaporation mixer was preheated at a temperature 20–50 °C above the fuel vaporization temperature, which was calculated from the Antoine equation [26]. To maximize the mixture homogeneity, the evaporation mixer was lengthened on the basis of a mixer used in our previous studies [27,28], and two net-shaped plates were added inside the cavity. Then the liquid fuel was pumped into the centerline of the air stream by the syringe pump. The mixer size could provide enough time to vaporize the fuel completely and ensured a fair homogeneity of the mixture. The equivalence ratio in the mixer could be altered by controlling fuel and air flow. The reformer was preheated to a specified temperature before preparation of the mixture. And then the homogeneous mixture was blown into the reformer. The equivalence ratio distribution without LTR was homogeneous in the reformer by CFD simulation. The reformer acted as a flow reactor, and it was composed of a stainless steel cavity (Φ40 mm × 490 mm) and a ceramic heating ring. A K-type thermocouple was mounted inside the cavity near the centerline of the outlet to record the reformer temperature. The temperature fluctuation was within a range of ± 10 K by a temperature controller. In this work, the reformer temperature was set to 473 K and 523 K respectively prior to pumping fuel. The simulated and measured temperature profiles along the reformer length using CFD modeling and a K-type thermocouple are shown in Fig. 2. It can be observed that the heating element produces an isothermal reaction zone with a temperature gradient in the vicinity of the inlet.

The engine operating conditions are listed in Table 2. All experimental results were obtained at an engine speed of 1200 rpm to ensure synchronization with the 10 Hz repetition rate of the laser. The intake air was heated to a temperature of 349 ± 0.5 K, and the intake temperature remained constant in the two reforming conditions. A common-rail system was used to provide an injection pressure of 600 bar. The fuel injection timing was −180 °CA ATDC (early injection). To ensure the safety of optical windows and the stable ignition, a relatively small amount of fuel (8 mg) was injected. In the operation, LTR products were blown into the intake port, and mixed with heated fresh air. Then the mixture was drawn into the cylinder to burn together with in-cylinder direct-injected fuel. The engine was kept supplied with LTR products at a steady flow. Then the whole system was in equilibrium when the engine worked at a certain speed, and the total amount of fuel participating in combustion was approximately the sum of