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Numerical study on the combustion and emission characteristics of a methanol/diesel reactivity controlled compression ignition (RCCI) engine

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HIGHLIGHTS

- ▶ Fuel reactivity can be well controlled by adjusting the methanol fraction and SOI.
- ▶ Appropriate methanol fraction and SOI contribute to the reduction of emissions.
- ▶ Both increased methanol fraction and advanced SOI are beneficial to fuel economy.
- ▶ Methanol addition is an effective way to achieve the efficient and clean combustion.
- ▶ Compared to diesel PCCI, methanol/diesel RCCI shows outstanding advantages.

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ABSTRACT

An improved multi-dimensional model coupled with detailed chemical kinetics mechanism was applied to investigate the combustion and emission characteristics of a methanol/diesel reactivity controlled compression ignition (RCCI) engine. The fuel was supplied separately by directly injecting diesel fuel into cylinder well before top dead center, while premixing methanol through the intake port in the tested methanol/diesel RCCI engine. The effects of mass fraction of premixed methanol, start of injection (SOI) of diesel and initial in-cylinder temperature at intake valve closing (IVC) on engine combustion and emission were investigated in detail. The results show that both methanol mass fraction and SOI have a significant impact on cetane number (CN) distribution, i.e. fuel reactivity distribution, which determines the ignition delay and peak of heat release rate (HRR). Due to larger area with high-temperature region and more homogeneous fuel distribution with increased methanol, and the oxygen atom contained by methanol molecule, all the emissions are reduced with moderate methanol addition. Advanced SOI with high combustion temperature is favorable to hydrocarbon (HC) and soot reduction, yet not to the decrease of nitrogen oxide (NO_x) and carbon monoxide (CO) emissions. Both increasing methanol fraction and advancing the SOI are beneficial to improve fuel economy and avoid engine knock. Moreover, it was revealed that the initial temperature must be increased with increased methanol fraction to keep the 50% burn point (CA50) constant, which results in decrease of the equivalent indicated specific fuel consumption (EISFC) and all emissions, except for slight increase in NO_x due to the higher burning temperature.

1. Introduction

With the development of the world economy, the demand for crude oil is growing rapidly. The researchers are more interested in the compression–ignition (CI) engines for its better fuel economy with high compression ratio and no throttling losses. But for the conventional CI engine, it suffers from high nitrogen oxides (NO_x) and particulate matter (PM) emissions. By providing low emissions while maintaining the high efficiency, the diesel premixed charge compression ignition (PCCI) attracts increasing attentions in recent decades [1–3]. In the PCCI combustion

Abbreviations: ATDC, after top dead center; BTDC, before top dead center; CA, crank angle; CO, carbon monoxide; CA10, 10% burn point; CA50, 50% burn point; CN, cetane number; DTBP, di-tert-butyl peroxide; DMCC, diesel/methanol compound combustion; EGR, exhaust gas recirculation; ERC, engine research center; EISFC, equivalent indicated specific fuel consumption; HRR, heat release rate; HC, hydrocarbon; HCCI, homogeneous charge compression ignition; IVC, intake valve closing; IMEP, indicated mean effective pressure; KH-RT, Kelvin Helmholtz–Rayleigh Taylor; NO_x, nitrogen oxide; PM, particulate matter; PCCI, premixed charge compression ignition; RCCI, reactivity controlled compression ignition; RNG, re-normalization group; RI, ringing intensity; SOI, start of injection; TDC, top dead center.

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strategy, PM can be reduced by promoting mixing of fuel and air prior to combustion. Meanwhile, NO_x is reduced by using lean fuel/air mixture as well as high exhaust gas recirculation (EGR) rate to cool the combustion temperature down. However, because of the low volatility and high flammability of diesel, there are still some problems yet to be solved for PCCI engine, including the formation of homogeneous mixture, ignition control, limited operating range, excessive wall impingement, and so on.

To overcome these problems associated with diesel PCCI combustion, the fuel reactivity controlled compression ignition (RCCI) has been proposed recently, which is an effective and clean combustion strategy by using two fuels with different properties and separate injection. The fuel with high octane number and low boiling point is injected into intake port, while diesel is injected into cylinder, so the stratified distribution of fuel reactivity is formed which leads to stratified combustion when be ignited by compression. The reduced heat release rate (HRR) caused by RCCI combustion resolves the engine knock when PCCI engine extends to high loads. The fuel of low boiling point is introduced through intake stroke, so the diesel that injected into cylinder directly becomes less, as a result, homogeneous mixture is easier to be implemented. In RCCI engine fueled with diesel, the ignition timing can be controlled by adjusting the proportion of diesel and other fuel and changing the start of injection (SOI). Inagaki et al. [4] conducted the related research by separate injection that iso-octane with high octane number was supplied into the intake port and diesel was injected into cylinder with significantly advanced injection timing. They found the ignition timing can be controlled by adjusting the proportion of two fuels, meanwhile high load extension can be achieved due to the low HRR caused by stratification of two fuels with different fuel reactivity.

Recently, the group led by Professor Reitz from the engine research center (ERC) of University of Wisconsin Madison conducted a series of studies on RCCI engine through experiment and simulation [5–8]. Kokjohn et al. [6] successfully controlled the ignition timing and HRR by adjusting fuel reactivity of gasoline injected into intake port and diesel injected into cylinder early. They pointed out that the diesel/gasoline RCCI engine can achieve 53% indicated thermal efficiency and meet the US-2010 regulations at low-to-medium load without any aftertreatment systems. Splitter et al. [7] described the non-homogeneous distribution of high reactivity and low reactivity mixtures in the cylinder by optical diagnostic experiments. The fuel stratification can prolong premixed combustion duration and achieve stratified combustion which is convenient to high load extension. Furthermore, Splitter et al. [8] realized the RCCI combustion through gasoline injected into intake port and the mixture of gasoline and a small amount of high-reactivity di-tert-butyl peroxide (DTBP) injected into cylinder. The results showed that the NO_x and soot emissions were comparable to the gasoline/diesel RCCI combustion, while the indicated thermal efficiency reached to 54% due to the reduced low-temperature HRR. Consequently, it was concluded that significant reactivity stratification can be formed to increase the RCCI combustion efficiency with only small amount of appropriate additives.

Compared to gasoline and diesel, methanol becomes the alternative fuel for its renewable and wide source that can be obtained from fossil and renewable sources, such as coal, petroleum, biomass, nature gas, wood and even ocean [9,10]. From the view of long run, methanol can enrich energy structure and satisfy people long-term development. From Table 1 [8,11], we can find the different properties of methanol, gasoline and diesel clearly. Moreover, methanol has a much higher latent heat of vaporization than gasoline and diesel, which can reduce combustion temperature effectively to restrict NO_x formation. Methanol has no carbon–carbon bonds, which is helpful to inhibit the soot formation. And it contains an oxygen atom which also contributes to hydrocarbon (HC), carbon monoxide (CO) and soot emissions oxidation. As a result, coping with the energy shortage and environmental challenge in the future, methanol shows greater potential and better adaptability.

Table 1
Properties of methanol, diesel and gasoline [8,11].

	Methanol	Euro-diesel	Gasoline
Formula	CH_3OH	$C_{12}H_{26}$–$C_{14}H_{30}$	C_4H_{10}–$C_{12}H_{26}$
Molecular weight (g/mol)	32	170–198	100–105
Density (g/cm^3, at 20 °C)	0.79	0.82–0.86	0.72–0.78
Boiling temperature (°C)	64.7	190–280	39–215.6
Flash point (°C)	11	52	−43
Auto-ignition temperature (°C)	470	300–340	257.2
Viscosity (mPa s at 298.15 K)	0.59	3.35	0.5–0.6
Stoichiometric fuel–air ratio	0.154	0.069	0.068
Cetane number	3–5	55	–
Lower heating value (MJ/kg)	20.27	42.74	43.2
Heat of vaporization (MJ/kg)	1.11	0.27	0.48

Seko and Kuroda [12] carried out a research about applying methanol on a single cylinder direct injection diesel engine with intake air heating. The parameters of SOI, intake temperature and exhaust gas recirculation (EGR) rate on combustion and emission characteristics were investigated to clarify the possibility of applying methanol to CI engine. They found that the methanol lean-burn system results in drastically NO_x reduction with almost the same brake specific energy consumption as diesel engine in the middle load. Xie et al. [13] also investigated the application of methanol on a Ricardo single cylinder port injection CI engine with large EGR rate and high intake air temperature, which performed well with low NO_x and HC emissions.

Despite methanol has its prominent advantage, methanol has a cetane number (CN) of about 3–5, which is much lower than that of diesel. Due to the low CN, auto-ignition is hard for methanol in engine combustion, especially in cold start and at light loads. The much higher latent heat of vaporization also weakens its auto-ignition ability. The lack of auto-ignition ability makes applying neat methanol to CI engine instead of diesel is still a challenge. Therefore, dual fuel with diesel and methanol was taken into account to take advantages of their respective characteristics. On account of the poor solubility of methanol in diesel, an additive has to be put into the mixture to form stable methanol/diesel blends, while the methanol fraction will not be too much. Chao et al. [14] performed a research of using methanol/diesel mixture with up to 15% of methanol by volume on a heavy-duty diesel engine. It was found reduction in NO_x and increase in HC and CO emissions with the increase of methanol. Huang et al. [15] conducted the similar research with up to 18% of methanol by weigh on a diesel engine, and found that when the methanol fraction was increased, the ignition delay became longer, and NO_x emission increased, while the CO and PM emissions decreased.

Sayin et al. [16] carried out relevant research on a methanol/diesel dual-fuel engine. The diesel fuel was blended with methanol to obtain four different fuel blends with methanol fraction ranging from 0% to 15% with an increment of 5% in volume ratio. Their results are consistent with those of Huang et al. [15]. In addition, the effect of three different SOIs of 15 °CA before top dead center (BTDC), 20 °CA BTDC and 25 °CA BTDC on emission characteristics was also discussed. It was revealed that, with advanced SOI, all of CO, HC and smoke emissions decreased, while NO_x increased.

Because of the poor miscibility of methanol and diesel, aiming at more effective reactivity control with more methanol supply, methanol and diesel can be supplied separately, i.e. methanol is delivered into the manifold and premixed with air, while diesel is injected into cylinder directly. Udayakumar et al. [17] used such fuel delivery strategy with intake air preheated to 70 °C on a