Fuel 213 (2018) 83–97

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Full Length Article

Numerical optimization and comparative study of n-butanol concentration stratification combustion and n-butanol/diesel reactivity stratification combustion for advanced compression ignition (CI) engine

Junhua Xiao[a], Ming Jia[a,*], Yachao Chang[a], Yaopeng Li[a], Zhen Xu[a], Guangfu Xu[a], Hong Liu[a], Tianyou Wang[b]

[a] Key Laboratory of Ocean Energy Utilization and Energy Conservation of Ministry of Education, Dalian University of Technology, PR China
[b] State Key Laboratory of Engines, Tianjin University, PR China

ARTICLE INFO

Keywords:
Reactivity stratification combustion (RSC)
Concentration stratification combustion (CSC)
Genetic algorithm
Multi-dimensional simulation
Combustion efficiency
Alternative fuels

ABSTRACT

Previous studies show that satisfactory engine performance can be achieved by using both the reactivity stratification combustion (RSC) and the concentration stratification combustion (CSC) fueled with n-butanol. However, the different ignition and combustion characteristics between RSC and CSC have not been well explored yet. In this study, the n-butanol/diesel RSC and n-butanol CSC strategies were compared by integrating the KIVA-3V code and the non-dominated sort genetic algorithm II (NSGA-II). For both RCS and CSC, n-butanol was premixed in the initial port. However, diesel and n-butanol were injected into the cylinder for RSC and CSC, respectively. Five important operating parameters were selected as the variables for optimization, including premixed fraction (PF), start of injection (SOI), the initial in-cylinder pressure at the initial valve close (IVC) timing, the initial in-cylinder temperature at the IVC timing (T_{ivc}), and exhaust gas recirculation (EGR) rate. The optimization results show that, for the realization of the clean and high-efficiency combustion, a wide range of SOI and the high PF are introduced in RSC, whereas a wide range of PF and the early SOI are employed in CSC. Due to the lower reactivity of n-butanol than diesel, CSC requires the higher T_{ivc} than RSC. As a fixed EGR rate, the optimal operating range of the initial temperature is restricted in a narrow range, especially for CSC. The optimal operating range of SOI and PF of RSC is larger than that of CSC.

In RSC, the homogeneous charge compression ignition (HCCI)-like combustion shows the lowest fuel consumption and NOx emissions, and the highest ringing intensity (RI). The reactivity control compression ignition (RCCI) combustion demonstrates the overall balanced engine performance. The benefit of the diesel induced ignition combustion on RI is evident, but the high NOx emissions are still a challenge. For CSC, the optimal case with the low concentration stratification of n-butanol achieves the good EISFC, the low NOx emissions, and the high RI. Generally, the RSC strategy is superior to the CSC strategy in terms of the control of combustion phasing, fuel efficiency, and emissions.

1. Introduction

It is acknowledged that internal combustion engines are the primary sources of air pollution and fossil fuel depletion. In response to the increasing energy crisis and the more stringent emission regulation, both improving the thermal efficiency and reducing the exhaust emissions simultaneously are imperative for internal combustion engines. Generally, conventional compression ignition (CI) engines demonstrate the higher thermal efficiency than spark ignition (SI) engines, with the penalty of higher nitrogen oxides (NO_x) and particulate matters (PM) emissions. Although the PM emissions of conventional CI engines can be reduced using the high injection pressure and the optimized combustion chamber, the NO_x emissions increase inevitably due to the high combustion temperature [1]. The NO_x emissions can be reduced by introducing the external exhaust gas recirculation (EGR), at the cost of the high fuel consumption.

In recent years, low temperature combustion (LTC) strategies were proposed to improve the trade-off relationship between the NO_x and soot emissions, as well as that between the NO_x emissions and fuel economy. Homogeneous charge compression ignition (HCCI) is one of the most representative combustion modes of LTC. For HCCI, the homogeneous fuel/air mixture is induced into the cylinder through the

* Corresponding author.
E-mail address: jiaming@dlut.edu.cn (M. Jia).

http://dx.doi.org/10.1016/j.fuel.2017.10.104
Received 26 June 2017; Received in revised form 10 September 2017; Accepted 24 October 2017
0016-2361/

Nomenclature

ATDC	After top dead center
CA50	50% heat release point
CDC	conventional diesel combustion
CFD	computational fluid dynamics
CI	conventional compression ignition
CO	carbon monoxide
CSC	concentration stratification combustion
EGR	exhaust gas recirculation
EISFC	equivalent indicated specific fuel consumption
EVO	exhaust valve opening
HC	hydrocarbon
HCCI	homogeneous charge compression ignition
HRR	heat release rate
IMEP	indicated mean effective pressure
IVC	initial valve close
LHV	lower heating value
LTC	low temperature combustion
NO_x	nitrogen oxides
NSGA-II	non-dominated sort genetic algorithm II
PCCI	premixed charge compression ignition
PF	premixed fraction
PM	particulate matters
PPRR	peak pressure rise rate
RCCI	reactivity control compression ignition
RSC	reactivity stratification combustion
SI	spark ignition
SOI	start of injection

Variables

p_{ivc}	initial in-cylinder pressure at the IVC timing
T_{ivc}	initial in-cylinder temperature at the IVC timing
τ_{inj}	injection duration

port injection of the fuel, and the auto-ignition occurs by the compression of the piston. Najt et al. [2] found that not only the ultralow soot and NO_x emissions, but also the comparable thermal efficiency to conventional diesel combustion (CDC) can be achieved by HCCI combustion. However, due to the dominant effect of the chemical kinetics on the combustion phasing in HCCI, the control of the ignition timing is extremely difficult. Meanwhile, owing to the multi-sites simultaneous ignition in the cylinder, the excessively high pressure rise rate and the rapid heat release restrict the engine operation to high loads [3]. It has been revealed that introducing the fuel concentration stratification and the fuel reactivity stratification into HCCI is beneficial to alleviate the fast combustion rate [4]. Thus, the premixed charge compression ignition (PCCI) combustion and the reactivity control compression ignition (RCCI) combustion are correspondingly proposed and are investigated extensively in recent years.

The fuel in PCCI is directly injected into the cylinder at an early crank angle during the compression stroke, and the partially premixed fuel/air mixture is formed before auto-ignition. Therefore, different from the rapid multi-sites combustion of HCCI, the PCCI combustion is more moderate along the gradient of the fuel concentration. The combustion of PCCI belongs to the concentration stratification combustion (CSC) strategy. The study of Lee et al. [5] indicated that the PCCI combustion inherits the advantages of HCCI combustion, but good fuel economy and low NO_x and soot emissions can also be obtained. According to different operating conditions, the in-cylinder fuel concentration stratification in PCCI can be varied through adjusting the start of injection (SOI) of the fuel, thus the burning rate can be effectively controlled.

Similar to the concentration stratification, the reactivity stratification is also beneficial to control the combustion phasing and reduce the combustion rate. The low-reactivity and high-reactivity fuels are respectively injected into the intake port and the cylinder, which is also named as RCCI combustion by Kokjohn et al. [6]. It is worth noting that the concentration stratification also exists in the cylinder in RCCI due to the direct in-cylinder fuel injection, although the reactivity stratification plays a more important role on the ignition and combustion process [7]. For convenience, it is simplified as reactivity stratification combustion (RSC) in this study.

Li et al. [8] studied the influence of premixed fraction (PF) and SOI on the performance of a methanol/diesel RCCI engine, the results indicated adjusting SOI and PF can effectively control the distribution of the fuel concentration and reactivity in the cylinder, so as to control the ignition and combustion processes. Recently, by optimizing bowl geometry, air handling, and fueling strategy, the potential of the extension of the RCCI operating conditions to low and high loads was well demonstrated by Kavuri and Kokjohn [9]. Although the RCCI combustion can achieve the good performance on the control of the ignition timing, the employment of two fuel supply systems makes the engine complicated. To clearly demonstrate the characteristics of the different combustion modes, the comparisons of the combustion modes mentioned above are listed in Table 1.

Gasoline and diesel are the most common fuels used in internal combustion engines. However, with the development of the fuel production technology, the application of the alcohol fuels to engines attracts increasing attentions. Compared to gasoline and diesel, alcohol fuels have several unique advantages, which are beneficial to realize the LTC strategy with the low exhaust emissions. First, alcohol fuel is renewable, which can be produced from the renewable feedstock, such as biomass, wood, and so on [10–12]. From the long-term perspective, alcohol fuel could enrich the energy structure and achieve the sustainable development. Second, both the high volatility and the high latent heat of vaporization can notably decrease the maximum combustion temperature in the cylinder and reduce the NO_x emissions. Moreover, the oxygen atom contained in the fuel molecule and the short chain length help to suppress the soot formation and enhance the fuel oxidation, as indicated in Refs. [13–15].

Methanol and ethanol are the most widely used alcohols, which have been applied in practical engines. However, the application of methanol and ethanol has several common drawbacks, which can be effectively avoided by n-butanol [16]. As listed in Table 2, compared to methanol and ethanol, the weaker water-absorbing characteristics and the higher flashing point of n-butanol decrease the corrosion effect of the storage tank and improve the security of both storage and transportation. Furthermore, the higher energy density of n-butanol supplies more sufficient power at high loads, and its lower latent heat of

Table 1
Summary of the characteristics of different engine combustion modes.

Combustion Mode	Characteristics
CDC	• Direct injection of the fuel into the cylinder around TDC
HCCI	• Injection of the fuel into the intake port
PCCI	• Direct injection of the fuel into the cylinder well before TDC
RCCI	• Injection of the low-reactivity fuel into the intake port • Injection of the high-reactivity fuel into the cylinder well before TDC
CSC	• Formation of the fuel concentration stratification in the cylinder by the fuel supplement strategy
RSC	• Formation of the fuel reactivity stratification in the cylinder by the fuel supplement strategy