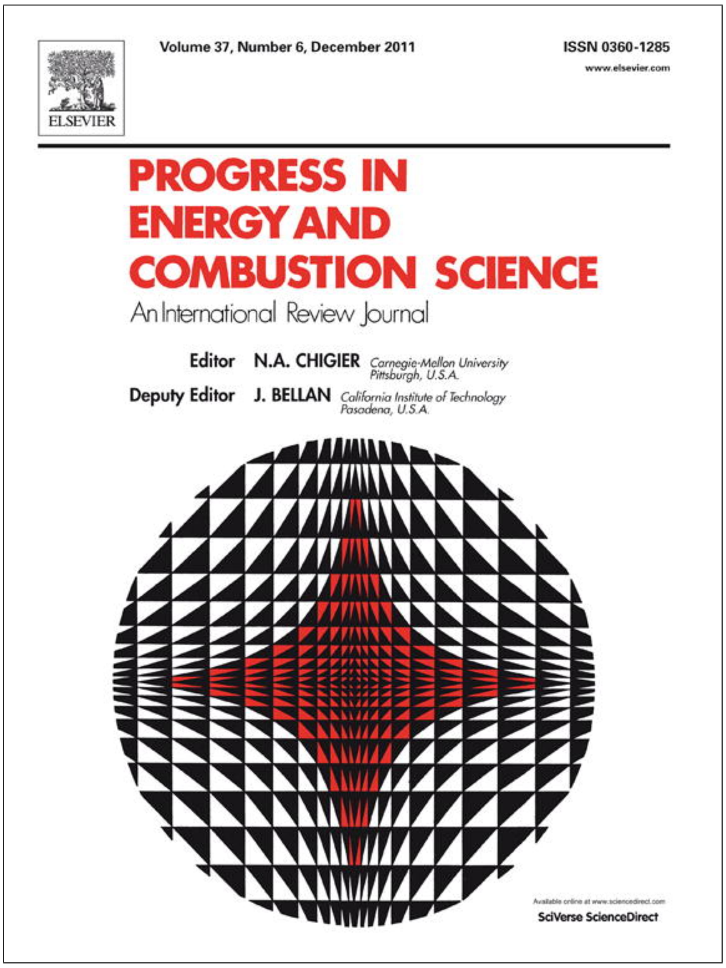

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Review

Fuel design and management for the control of advanced compression-ignition combustion modes

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ABSTRACT

Due to concerns regarding the greenhouse effect and limitations on carbon dioxide emissions, the possibility of a next-generation combustion mode for internal combustion engines that can simultaneously reduce exhaust emissions and substantially improve thermal efficiency has drawn increasing attention. The most prominent characteristic of new combustion modes, such as Homogenous-Charge Compression-Ignition (HCCI), Stratified-Charge Compression-Ignition (SCCI), and Low-Temperature Combustion (LTC), is the requirement of creating a homogenous mixture or controllable stratified mixture prior to ignition. To this end, a lean fuel/air mixture and/or a controllable high level of exhaust gas recirculation (EGR) are employed to prolong the timescale of the ignition chemistry and port fuel injection or early in-cylinder injection is used to lengthen the mixing period. The mixture then undergoes controlled self-ignition near the top dead center (TDC) position due to the compression effect of the piston's upward movement. It is worth noting that the entire combustion process lacks a direct method for the control of ignition timing and combustion rate, which are instead controlled primarily by chemical kinetics and, to a lesser extent, by turbulence and mixing. Because of the significant impacts of fuel physical–chemical properties on the ignition and combustion process, fuel design and management has become the most common approach for the control of ignition timing and combustion rate in such advanced combustion modes.

This paper summarizes the concepts and methods of fuel design and management and provides an overview of the effects of these strategies on ignition, combustion, and emissions for HCCI, LTC, and SCCI engines, respectively. From part 2 to part 4, the paper focuses on the effect of fuel design on HCCI combustion. A fuel index suitable for describing ignition characteristic under HCCI operating conditions is first introduced. Next, the proposed fuel design concept is described, including principles and main methodologies. Strategies based on the fuel design concept (including fuel additives, fuel blending, and dual-fuel technology) are discussed for primary reference fuels (PRF), alternative fuels, and practical gasoline and diesel fuels. Additionally, the effects of real-time fuel design on HCCI combustion fueled with PRFs and dimethyl ether/liquefied petroleum gas (DME–LPG) are evaluated. Diesel HCCI combustion has suffered from difficulties in homogenous mixture formation and an excessively high combustion rate. Therefore, LTC, which concentrates on local combustion temperature and a balance of mixture formation timescale and ignition timescale, has been proposed by many researchers. In Part 5, this paper provides an overview of the major points and research progress of LTC, with a preliminary discussion of the fundamental importance of fuel properties and fuel design strategy on the LTC process and emissions. Due to the stratification strategy has the capable of extending the HCCI operation range to higher loads, SCCI combustion, which incorporates HCCI combustion into a traditional combustion mode, has the potential to be used in commercial engines. Thus, this paper discusses the principles and control strategies of fuel design and management and also summarizes recent progress and future trends. The effect of fuel design and management on SCCI combustion is assessed for high cetane number fuels and high octane number fuels as well as the in SCCI combustion of gasoline–diesel dual-fuel and blends.

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Contents

1. Introduction

Internal combustion engines are the primary power sources for transport vehicles, marine ships, construction equipment, and agricultural machineries, among others. Engines consume extremely large amounts of fuel to produce power and emit poisonous or harmful exhaust gases, which include CO, HC, NO*x*, particulate matter (PM), and CO_2. Over the past two decades, worldwide research in the engine and automotive industries has been dedicated to engineering higher fuel efficiency and lower emissions as well as the development of renewable alternative fuels due to the finite amount of fossil fuels. However, existing emission reduction technologies have improved engine-out emissions at the expense of lower fuel economy. As a result, the thermal efficiency of engines has not improved significantly despite the rapid progress in the automotive industry and manufacturing engineering fields. This situation exacerbates the shortage of vehicle fuels and increases the gross amount of greenhouse gas emissions.

Improving energy utilization while minimizing all types of pollutants has became a key scientific target in the field of internal combustion engines. Moreover, because of rising concerns about the greenhouse effect over the past few years, several governments and organizations have introduced peremptory legislative standards of fuel economy. Recently, legislation regarding CO_2 emissions from passenger cars was officially published in the form of Regulation (EC) No 443/2009 of the European Parliament and the Council of 23 April 2009, setting emissions performance standards for new passenger cars as part of the Community's integrated approach to the reduction of CO_2 emissions from vehicles. The fleet average that must be achieved by all cars registered in the EU is 130 g/km in 2012, and 65% of each manufacturer's newly registered cars must comply with the limit value curve set by this legislation. This figure will rise to 75% in 2013, 80% in 2014, and 100% from 2015 onwards. At the same time, other emissions, including HC, CO, NO*x*, and PM, will most likely be required to meet more severe future standards, such as those of EURO V. Additionally, America, Japan, China, and several other countries have also issued more stringent fuel economy and emissions standards.

Some researchers have indicated that the fuel economy of traditional piston engines has the potential for further improvement by 25% or more (while reducing harmful emissions to approximately zero) by supplementation with advanced combustion technology. For this reason, global researchers have paid more attention to advanced combustion modes. Among these, HCCI, SCCI, and low-temperature combustion modes are featured as possibilities for use in compression–ignition engines. Because of their extremely low NO*x* and PM emissions as well as their relatively high thermal efficiencies, these examples are commonly recognized as next-generation combustion modes separate from conventional spark ignition (SI) and direct injection compression ignition (DICI) combustion modes. The initial concept of HCCI combustion was based on a combination of the advantages of SI and DICI engines while avoiding their disadvantages. This mode operates with a leaner homogenous mixture but is autoignited near TDC by piston compression. In the case of LTC, an overall uniform in-cylinder mixture is not desired; instead, the mode focuses on local mixture preparation and local/global combustion temperature by balancing the required physical timescale of local mixture formation with the ignition chemistry timescale. PM and NO*x* formation is minimized by controlling both the global temperature as well as the local temperature in the cylinder. SCCI combustion attempts to leverage the advantages of HCCI combustion for commercial engines by integrating traditional and advanced combustion modes. To some extent, LTC and SCCI are inspired and furthered by the concept of HCCI, and can be regarded as further developments of the HCCI combustion concept.

HCCI combustion has been considered a promising alternative combustion mode for SI and DICI engines since the end of the 1990s. Since then, it has received wide financial support from governments, organizations, and companies in the USA, Europe, and Asia for the research and development of next-generation engine power. Published documents illustrate that HCCI combustion can be scaled for use in virtually every size-class of transportation engines with all practical fuels and potential alternative fuels and that it is a good prospective combustion approach because it has inherently low NO*x* and PM emissions but relatively high thermal efficiency. In addition, HCCI combustion is considered to be an indispensable technology for meeting increasingly stringent standards for exhaust emissions (such as Euro VI) and potential regulations regarding CO_2 emissions worldwide.

1.1. HCCI operating principle

Due to existing obstacles in traditional SI and DICI engines, HCCI combustion was proposed as a novel engine operation strategy at the end of the 1970s. In fact, the most recognized original work on HCCI by Onishi et al. [1] and Noguchi et al. [2] was motivated by a desire to control the irregular combustion caused by auto-ignition of the cylinder charge in order to obtain stable lean-burn combustion in the conventionally-ported two-stroke gasoline engine. The apparent potential of this active thermo-atmosphere combustion (ATAC) process for the reduction of emissions and fuel consumption, coupled with serious shortfalls of the ported two-stroke engine as an automotive power unit, led to an investigation into the application of this new combustion process to a four-stroke single-cylinder engine by Najt and Foster in 1983 [3]. In 1990, the idea of hot premixed combustion in a diesel engine was proposed by Hu et al. [4] and is considered one of the pioneering works in diesel HCCI combustion.

Over the last two decades, various names have been assigned to this new combustion process, including ATAC (Active Thermo-Atmospheric Combustion), TS (Toyota-Soken), ARC (Active Radical Combustion) for conventional two-stroke engines, CIHC (Compression-Ignited Homogeneous Charge), HCCI (Homogeneous-Charge Compression-Ignition), CAI (Controlled Auto-Ignition), UNIBUS (Uniform Bulky Combustion System), PREDIC (PREmixed lean Diesel Combustion), PCI (premixed compression ignition), MK (Modulated Kinetics), PCCI (Premixed-Charge Compression-Ignition), and OKP (Optimized Kinetic Process) in four-stroke engines.

The fundamental goal of HCCI combustion is the combination of the advantages of SI and DICI engines and the avoidance of their disadvantages. A conventional SI engine employs a homogenous fuel/air mixture that is mixed in the intake port and then undergoes induction compression. Engine load is controlled by adjusting the throttle, and the fuel/air mixture is ignited by spark discharge. It features extremely low soot emission but also has lower thermal efficiency due to pumping loss and a low compression ratio, which is limited by knocking combustion. In contrast, a traditional DICI engine employs a heterogeneous fuel/air mixture. It directly and rapidly injects fuel into the combustion chamber near TDC, which is then self-ignited after a short delay time. Therefore, there is less pumping loss, and the high compression ratio generates higher efficiency; the disadvantages to this method, however, are the high levels of NO*x* and soot and the trade-off relationship.

In contrast, HCCI combustion is achieved by controlling the temperature, pressure, and composition of the lean homogenous air/fuel mixture so that it auto-ignites at multiple points and subsequently reacts homogeneously as it is compressed by upward piston movement. For neat HCCI combustion, the heat release reaction is distributed throughout the combustion chamber without flame propagation and local high-temperature zones or rich-fuel zones. Thus, a uniform mixture and average low-temperature limit the production of NO*x* and PM. In this combustion mode, the mixture temperature is the most important parameter, and it plays a significant role in determining combustion characteristics and emissions for several reasons. First, the high-temperature chemical reaction or self-ignition occurs only if the mixture temperature exceeds the auto-ignition threshold. Second, ideally the maximum combustion temperature should exceed 1500 K so as to ensure the completed oxidation from CO to CO_2. Finally, the maximum temperature should be kept lower than the critical temperature of NO*x* formation.

1.2. Advantages and challenges of HCCI combustion

Table 1 provides a brief comparison of the basic features of HCCI, SI, and DICI combustion and summarizes several benefits of the HCCI engine as follows [5]:

- HCCI combustion employs a higher compression ratio, lacks a threshold value, and features shorter combustion duration and a fast combustion rate. Thus, it approximates constant-volume combustion and achieves a higher thermal efficiency

Table 1
Comparison of traditional combustion modes and HCCI combustion.

	SI	DICI	HCCI
Fuel	Gasoline-like fuels	Diesel-like fuels	Flexible fuel
λ	≈ 1.0	$=1.2–2.2$	>1.0
Mixture preparation	PFI, GDI	DI	DI, PFI, and DI + PFI
Ignition	Spark ignition	Auto-ignition	Auto-ignition
Combustion form	Premixed	Diffusion	Premixed but dominated by chemical kinetics
Combustion rate limitation	Flame propogation	Mixing rate	Multipoint or spontaneous
Flame front	Y	Y	w/o
Combustion temperature	High	Partially high	Relatively low

due to the lower combustion temperature and lower radiation loss.

- There is no flame front or flame spread or local areas of excessively high temperature and rich mixture and, thus, there is no soot production. Furthermore, given the low-temperature condition and uniform distribution of the bulk gas temperature, NO*x* emissions can also be restricted to a low level.
- The third advantage of HCCI combustion is fuel flexibility. This feature could alleviate dependence on petroleum resources by enabling the use of various alternative fuels [6,7,8].

The control of HCCI combustion is fundamentally more challenging than using a direct control mechanism such as a spark plug or fuel injector to dictate ignition timing, as in SI and CIDI engines. Nonetheless, HCCI engines have several inherent benefits as potential replacements for SI and CIDI engines in vehicles with conventional powertrains. HCCI has thus far been incorporated in certain production DI diesel engines, enabled not only by a better understanding of the physical and chemical processes involved in this combustion mode but also by discovery of technical solutions for practical applications of this new combustion mode. The main obstacles that have kept HCCI from being applied to commercial engines can be stated as follows [5,9]:

(1) Ignition timing control over wide engine speed-load ranges: It is widely recognized that HCCI combustion is driven by chemical kinetics and is therefore controlled by fuel physical–chemical properties as well as the temperature history of the fuel/air mixture. On the contrary, in-cylinder turbulence and mixing have little influence on combustion timing. As the ignition timing has been shown to be very sensitive to factors such as octane number, intake charge temperature, fuel/air equivalence ratio, mixture composition or EGR rate, and fuel composition, the most pressing task for HCCI implementation is to ensure that ignition occurs near TDC under variable working conditions.

(2) Combustion rate control from high- to full-load engine operation: HCCI combustion has been demonstrated to operate well at low to medium loads but difficulties have been encountered at high loads. Combustion can become very rapid and intense, causing unacceptable noise, potential engine damage, and eventually, unacceptable levels of NO*x* emissions. Additional work is needed to develop methods that reduce the heat release rate under high-load operation conditions to prevent excessive noise or engine damage.

(3) Cold start capacity: HCCI ignition is very sensitive to intake charge temperature, and minor variations alter combustion phasing significantly. Furthermore, the initial temperature required to achieve self-ignition varies with fuel properties and operation conditions. Under cold start and idle operating conditions, the compressed gas temperature will be reduced because the charge receives no preheating from the intake manifold and is rapidly cooled by heat transferred to the cold combustion chamber walls. Without some compensatory mechanism, low compressed charge temperatures could prevent an HCCI engine from firing.

(4) Higher levels of HC and CO: HCCI combustion produces inherently low emissions of NO*x* and PM at lower engine loads but relatively high emissions of HC and CO at low to medium loads as well as high emissions of NO*x* under large loads. Thus, it is necessary to develop emission control systems and control strategies to overcome the challenge of excessive HC and CO emissions, particularly at low loads.

(5) Mixture preparation: This is particularly important for poor volatility diesel-fueled HCCI combustion. The main goals here are to avoid wall impingement, to promote fuel vaporization and air mixing so as to limit PM and HC emissions, and to prevent oil dilution.

(6) Prompt response of cycle transient: HCCI lacks a real-time, rapid-response control system to overcome the challenge of maintaining proper ignition timing during rapid variations in engine speed and load.

(7) Engine control strategies and systems: Additional work is needed with regards to the development of a new methodology for feedback and closed-loop control of fuel and air systems, advanced control theory and control arithmetic, next-generation combustion sensors, and next-generation software and hardware specialized for HCCI combustion in order to optimize combustion over wide load-speed ranges.

(8) Cylinder-to-cylinder variation: Theoretical studies and fundamental experiments have been conducted mostly on single-cylinder engines. However, when HCCI was applied to multi-cylinder engines, the residual gas fraction, intake charge temperature, mass and composition of the fuel, and air charge were observed to differ to some extent because of the structure and length of the manifolds. These small differences can cause the ignition timing and combustion rate to vary greatly. As a result, misfires may be observed in certain cylinders, whereas serious knock or detonation may occur in other cylinders. Therefore, research and development (R&D) is needed to produce intake and exhaust manifold designs for multi-cylinder engines to overcome the challenge of maintaining strict uniformity of the inlet and exhaust flows on each cylinder.

(9) Relatively higher pressure-rise rate and severe combustion noise: Because the HCCI combustion rate is so high, ignition occurs simultaneously throughout the combustion chamber, producing a high pressure-rise rate and high-frequency noise or intensive ringing when compared to the behavior of a conventional DICI or SI engine, especially under a large equivalence ratio [10].

(10) Accurate chemical mechanism and precise combustion model: During the R&D process, a large number of design proposals and research strategies rely on numeric calculations and

Table 2
Papers related to HCCI combustion over the past ten years (ISI indexed & SAE papers).

	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010
SAE papers	8	24	42	50	60	90	68	85	92	76	54
ISI indexed papers	3	2	10	16	20	53	49	91	76	90	65

simulations. To accurately predict specific features and emission levels in the HCCI combustion process, it is necessary to develop a multi-dimensional CFD combustion model that is coupled with detailed chemical kinetics in order to overcome the challenge of rapidly and inexpensively evaluating engine geometry and combustion system designs.

1.3. Overview of HCCI research activities

In the late 1990s, European countries, the USA, and Japan conducted aggressive research and development programs in the area of HCCI, including both public and private sector components and universities. Many of the leading HCCI developments to date have come from these countries, at institutions such as Lawrence Livermore National Laboratory, Sandia National Laboratory, University of Michigan, Lund University, Brunel University, Keio University, etc. Their work has produced constructive contributions to a deeper understanding of HCCI operation principles.

Accordingly, published papers related to HCCI combustion from international conferences and in technical journals have increased greatly, as shown in Tables 2 and 3. For instance, only eight papers related to HCCI combustion were reported in the 2000 SAE Congress. Since then, due to renewed interest in HCCI combustion, the HCCI session at the annual SAE Congress has become one of the most active sessions, gathering the most researchers and R&D engineers at the 2002 event. Thereafter, with the increase in the quantity of HCCI papers, Society of Automotive Engineers (SAE) has released at least one special issue focusing on HCCI each year. For example, in 2005, SP-1963 released 48 papers, and in 2006, SP-2005 published 49 articles. From 2007 to 2009, special issues on HCCI included approximately 40 articles each year on this topic. Additionally, an increasing number of institutes, companies, and universities have joined the effort to carry out fundamental and applied research on HCCI combustion. In particular, many oil companies have also gained insight into fuel flexibility and fuel requirements for HCCI combustion. Thus, some excellent work and data have been reported at the annual conference of Fuel and Lubrication.

There is no direct control strategy for ignition timing in HCCI, in which ignition is primarily determined by fuel/air mixture properties as well as temperature-history, boundary conditions, and operation conditions. As a result, HCCI combustion is characterized by cyclic fluctuations, unstable combustion, misfire, knock, and incomplete combustion, which greatly constrain the operation range of HCCI. Therefore, the most challenging task facing HCCI combustion is the control of ignition timing and burn rate. Published documents indicate that many factors may influence

Table 3
Categories and main contents in SP regarding HCCI (published by SAE from 2001 to 2010).

Research aspects	Paper numbers	Research contents	Main research unit
Gasoline HCCI	78	Residual gas trapping and its control, external EGR, camless HCC engine, load expanding, mode switching, GDI based HCCI, cyclical fluctuation, SCCI, spark-assisted self-ignition	Brunel University, Lund University, University of Birmingham, Ford, GM, Stanford University, University of Cambridge, Jugar, Tsinghua University, AVL, Tianjin University, etc.
Diesel HCCI	45	External EGR, load extension, fuel-supplying strategy, influence of combustion chamber boosting, VVT, VCR, PCCI, mixture preparation	University of Wisconsin Madison; National Traffic Safety and Environment Laboratory, University of Michigan, Sandia National Lab, New ACE, Toyota, Tianjin University, Shanghai Jiao Tong University, Southwest Research Institute, IFP, Lund University, etc.
Alternative fuel HCCI	25	Natural gas, Ethanol, methanol, hydrogen, DME	Shanghai Jiao Tong University, Keio University, Korea Advanced Institute of Science and Technology, Lund University, Tianjin University, University of California Berkeley, etc.
Theoretical study	108	Mixture and temperature distribution, fuel design, closed-loop control, heat transfer of boundary layer, effect of compression ratio, chemical kinetics, VCR, EGR mechanism, Heat management, cyclical fluctuation, gas reforming, analysis of emission components, measurement of in-cylinder temperature and emission formation, measurement and control of combustion process	Shanghai Jiao Tong University, Keio University, Lund University, Lawrence Livermore National Lab, Sandia National Lab, University of Michigan, University of California Berkeley, etc
Optical diagnostic	22	PLIF research on boundary layer reaction, PLF and chemoluminescence, Mixture distribution, ignition mechanism, combustion process, pollutants formation and evolution	Brunel University, Lund University Sandia National Lab, Stanford University, University of Illinois at Urbana-Champaign, etc
Numeric simulation	61	Multi-zone model, Ignition prediction with detail chemical kinetics, multi-dimension CFD coupled with detail chemical kinetics, sequential CFD-multi-zone chemical kinetics, Detail chemical kinetics with gas exchange process, Large eddy simulation, direct numerical simulation	University of Wisconsin Madison, Ricardo, Tianjin University, Brunel University, University of Michigan, Tsinghua University, University of California Berkeley, etc

ignition, combustion, and pollutant formation throughout the engine time history, including fuel properties, the main pathways of elementary reactions and their reaction rates, mutual interference of multi-components, and coupling effects between fuel molecular and residual gas fractions. Additionally, physical properties such as boiling point, viscosity, distillation history, surface tension, and the latent heat of evaporation also play a significant role in the required timescale for homogenous mixture formation. Thus, fuel properties are important factors in ignition timing control and load extension for HCCI combustion.

For practical operation cases, where boundary conditions vary from cycle-to-cycle and from cylinder-to-cylinder, fuel properties with fixed components were unable to meet the requirements of proper combustion phasing, load expansion, emission optimization, and maximum thermal efficiency in HCCI combustion. Therefore, the influence of fuel chemistry on HCCI and the control of the combustion process by fuel design have become one of primary directions in HCCI investigation. From this background, this paper systematically generalizes the research progress and future trends in new-generation combustion modes (including HCCI, LTC, and SCCI) based on fuel design theory and methods. In a sense, this review is a partial update of previous, more comprehensive reviews conducted in order to account for recent investigations that have led to important progress in HCCI combustion control via fuel design in primary reference fuels, alternative fuels, and fossil fuels. However, we also concentrate on two important advanced compression-ignition combustion modes, namely, LTC and SCCI, and their operating principles; we also discuss new evolutions in ignition and combustion control stemming from fuel design and management.

2. Principle of fuel design for control of HCCI combustion

2.1. General oxidation chemical kinetics of hydrocarbon fuels

Advanced combustion concepts that rely on compression self-ignition have demanded an improved understanding of the detailed mechanisms of hydrocarbon chemical kinetics, particularly in the low-temperature oxidation regime, as well as fuel effects on auto-ignition. Moreover, the increasing use of alternative and nontraditional fuels presents new challenges for combustion modeling and demands accurate rate coefficients and branching fractions for a wider range of reactants. More comprehensive and well-documented reviews of the detailed chemical kinetic models for low-temperature oxidation mechanisms – including reactions of alkyl radicals, ethers and (methyl and ethyl) esters, alkenes, cycloalkanes, and aromatic compounds – have been published by Battin-Leclerc [11] and Zádor et al. [12]. Simmie et al. also reviewed detailed chemical kinetic models for intermediate- to high-temperature oxidation, ignition, and the combustion of alkanes, cycloalkanes, alkenes, and aromatic compounds [13]. In fact, modeling of low to medium temperature oxidation of hydrocarbons represents the foundation of the thermokinetic processes of auto-ignition [14–16]. These processes are relevant to the onset of 'knock' in spark-ignition engines. To gain valuable insights into the nature of knocking combustion in SI engines, Griffiths provided a summary of a reduced kinetics model specifically developed for the low-temperature regime and attempted to apply it in a practical combustion system [17]. Fuel components, carbon numbers, and molecular structure were observed to determine the oxidation mechanism and to sequentially dominate the ignition timing, combustion rate, and pollutant formation in a practical combustion subsystem. Regarding HCCI combustion, the development of comprehensive, detailed mechanisms for hydrocarbon oxidation has focused attention on certain aspects of HCCI combustion phenomena, including ignition, burn duration, intermediate species, and pollutant formation and evolution, in which the details of the chemistry are most important. Thus far, for practical hydrocarbon fuels with carbon numbers less than seven as well as for some important surrogate fuels, detailed and semi-detailed chemical kinetics have been widely modeled and validated on the basis of experimental results from rapid compression machines (RCM), shock tubes, jet-stirred reactions (JSR), flow reactors, and motored engines. These fuels include n-heptane [18–27], iso-octane [25–35], pentane [36–40], hexane [41,42], methane [43], dimethyl ether [44–48], propane [49], methanol [50], ethanol [51], dimethyl methane (DMM) [52], and methyl tert-butyl ether (MTBE) [53,54].

The vast majority of transportation fuels are composed of linear and branched hydrocarbons, and much emphasis has been placed on the study of n-heptane and iso-octane. The reason for this focus is that n-heptane and iso-octane are primary reference fuels (PRFs) for spark-ignition internal combustion engines. Additionally, they are often used as surrogate fuels for diesel fuel and gasoline in numerical simulation research. Therefore, a better understanding of the detailed chemical kinetics of PRFs and their mixtures under engine-like conditions is helpful for the control of HCCI ignition timing and burn rate. Curran et al. developed a detailed chemical kinetic mechanism with 544 species and 2446 elementary reactions in order to model the oxidation of n-heptane. This regime covered the initial ranges of pressure from 1 to 42 atm, temperature from 550 to 1700 K, equivalence ratio from 0.3 to 1.5, and nitrogen–argon dilution from 70 to 99% [20]. In 2002, Curran et al. released a detailed chemical kinetic mechanism with 860 species and 3600 elementary reactions to model the oxidation of iso-octane. Over the series of experiments investigated, the initial pressure ranged from 1 to 45 atm, temperature from 550 to 1700 K, equivalence ratio from 0.3 to 1.5, and nitrogen–argon dilution from 70% to 99% [28]. The aforementioned mechanisms have been widely accepted and show good agreement with the ignition delay measured on JSR, RCM, shock tubes, and practical engines. In addition, Buda et al. proposed a unified model with a single set of kinetic parameters for modeling the auto-ignition delay times of a wide range of alkanes using detailed kinetic mechanisms automatically generated by EXGAS software. The investigated conditions in this study cover the temperature range from 600 to 1200 K, including the negative temperature coefficient (NTC) region, a pressure range from 1 to 50 bar, and equivalence ratios from 0.5 to 2 [55]. Ranzi et al. constructed a detailed mechanism for iso-octane oxidation and validated it by measuring the ignition delay in a shock tube, RCM, flow reactor, and JSR [56].

Ignition is related to the presence of a dominant chain-branching reaction mechanism that can drive a chemical system reaction to completion in a very short period of time. Three major chain-branching regimes have been identified, one consisting of high-temperature ignition with a chain-branching reaction mechanism based on the reaction between atomic hydrogen and molecular oxygen, and others based on low to intermediate temperature thermal decomposition of hydrogen peroxide. In general, for alkanes with carbon numbers larger than four containing only C–C but no C=C bonds, the overall oxidation history can be divided into three regions: low temperature (less than 850 K), intermediate temperature (above 850 K but below 1200 K), and high temperature (above 1200 K).

At low temperature, the reaction is initiated by the abstraction of a hydrogen atom (H-abstraction) from the alkane by oxygen (O_2) molecules to yield alkyl and hydroperoxy radicals. These reactions are endothermic and are difficult to characterize experimentally, partly because they are slow reactions and partly because reactions of the products rapidly overwhelm the main reaction [11]. Alkyl radicals react rapidly with O_2 molecules to yield peroxyalkyl radicals (RO_2), leading to the formation of peroxide species and small radicals, which then react with alkane molecules by metatheses to regenerate alkyl radicals. After that, RO_2 radicals isomerize to produce a QOOH radical species. QOOH species react via several alternative paths, which are formally chain-propagation steps, but a second O_2 molecule adds preferentially to QOOH, creating a radical O_2QOOH, which can then isomerize further during the low-temperature period. The isomerized product decomposes into a relatively stable ketohydroperoxide species and one OH radical. The ketohydroperoxide species then possesses its own temperature for decomposition at about 800 K, somewhat lower than that of H_2O_2. Upon reaching this temperature, the ketohydroperoxide decomposes into several species, at least two of which are radicals [12]. Thus, it is not until this final ketohydroperoxide decomposition step that chain branching is finally achieved in the low-temperature oxidation regime. Because at least three of the ultimate products of this reaction sequence are radicals, chain branching becomes quite strong once the ketohydroperoxide decomposes. These degenerate branching steps involve a multiplication of the numbers of radicals, which induces an exponential acceleration of reaction rates in a chain reaction, leading to spontaneous auto-ignition in some cases [13].

As the temperature increases, the alkylperoxy radical becomes thermally unstable and can suffer a number of fates with differing consequences for the progress auto-ignition. Of course, the ROO radical can simply dissociate back to form the alkyl and O_2 reactants, removing the ROO chain carrier and “undoing” the initial reaction. Secondly, the ROO can produce HO_2 and the conjugate alkene. As HO_2 is relatively un-reactive and its removal reactions primarily produce H_2O_2 (which is stable up to 1100 K), this channel effectively chain-terminates at low temperatures. The emergence of this channel and the loss of the ROO chain carrier are partially responsible for the decreased reactivity with increasing temperature behavior observed for many hydrocarbons. This means that, when the temperature increases to the point at which it benefits the formation of alkenes (up to 850 K), a reduction of the overall reaction rate occurs, leading to the appearance of the negative temperature coefficient (NTC) regime. This distinctive feature of hydrocarbon oxidation signifies a temperature zone in which the global rate of the reaction decreases with an increase in temperature.

As the mixture temperature further increases, up to about 1050–1100 K, a hot flame is triggered by the decomposition of H_2O_2, a chain-branching reaction and forms two OH radicals [19]. The high-temperature oxidation mechanism of hydrocarbons can be simplified into three steps: 1) the alkyl radical combination with molecular oxygen at low temperature is changed to a decomposition reaction that forms small olefins and further oxidizes to CO and water under high temperature, 2) fuel molecular is directly cracked to small molecules with a small attendant heat release, and 3) further CO oxidization to CO_2 is accompanied by a large heat release. At temperatures above 1200 K, the dominant chain-branching step in hydrocarbon ignition consists of the consumption of one H atom by molecular oxygen, which produces two radicals, and H atoms that are produced by thermal decomposition of radicals such as ethyl, vinyl, formyl, and isopropyl.

Real fuels are complex mixtures of thousands of hydrocarbon compounds, including linear and branched paraffins, naphthenes, olefins, and aromatics. It is generally agreed that their behavior can be effectively reproduced by simpler fuel surrogates containing a limited number of components. More recently, Mehl et al. developed an improved version of the kinetic model to analyze the combustion behavior of several components relevant to gasoline surrogate formulation [57]. Particular attention is devoted to linear and branched saturated hydrocarbons, olefins (1-hexene), and aromatics (toluene). Westbrook et al. proposed a detailed chemical kinetic reaction mechanism for primary reference fuel mixtures of n-hexadecane and 2,2,4,4,6,8,8-heptamethyl nonane for diesel cetane ratings [58]. These reaction mechanisms are validated by comparisons between computed and experimental results for shock tube ignition and for oxidation under JSR conditions. Representative applications of this mechanism to several test problems are considered, describing fuel/air auto-ignition variations with changes from pure 2,2,4,4,6,8,8-heptamethyl nonane (cetane number of 15) to pure n-hexadecane (cetane number of 100).

It should be pointed out that, although the detailed chemical kinetics of many hydrocarbons include a low-temperature reaction regime, negative temperature coefficient zone, and high-temperature reaction regime, the major reaction pathways, elementary reaction rate, key intermediate products and formation routes, and reaction sensitivity depending on temperature history exhibit significant differences for different fuels. As a result, practical combustion systems show differences in intermediate products, active radicals and their concentrations, pollutant formation and evolution process, and fuel consumption history. In the engine combustion system, this results in different ignition phasing, heat release patterns, burn duration, pollutant species, and concentrations.

2.2. Basic characteristics of HCCI combustion

Fig. 1 shows the in-cylinder pressure, heat release curve, and temperature-time history for a classic HCCI combustion event. The HCCI combustion clearly exhibits two-stage heat release, including a low-temperature heat release (LTHR, also referred to as low-temperature reaction, cool-flame, or first-stage combustion) and a high-temperature heat release (HTHR, also known as high-temperature reaction, hot flame, or second-stage combustion). The basic characterization parameters of the low-temperature reaction are defined in the figure: initial onset of the LTR (SOI_{LTR}), initial temperature corresponding to SOI_{LTR} (T_{LTR}), maximum heat release rate during the LTR ($HRR_{LTR,max}$) and its corresponding crank angle ($\theta_{LTR,max}$), cumulative heat release during the LTR, end crank angle of the LTR, temperature rise during the LTR (dT_{LTR}), and reaction duration of the LTR (BD_{LTR}). The characterization parameters of high-temperature combustion include the onset of HTR (SOI_{HTR}), initial temperature corresponding to SOI_{HTR} (T_{HTR}), maximum heat release rate in the HTR ($HRR_{HTR,max}$) and its corresponding crank angle ($\theta_{HTR,max}$), burn duration of HTR (BD_{HTR}), and induction timing (ID_{HTR}) between the LTR and HTR. Furthermore, parameters such as the maximum in-cylinder pressure (P_{max}), maximum combustion temperature (T_{max}), and maximum pressure-rise rate (PRR_{max}) are also used to characterize the engine performance.

It is obvious that the low-temperature reaction has a significant influence on the high-temperature reaction. Many factors directly determine the characteristics of the LTR and HTR, including elementary reaction rate, intermediate products and their concentrations, active radicals and their formation, and termination. From the point of view of chemical kinetics, many hydrocarbon fuels exhibit two-stage reactions and NTC phenomena, but the apparent characteristics of HCCI combustion show remarkable variation with different fuels.

For practical engine combustion, the mixture ignition timing, combustion rate, and combustion efficiency are not only dominated by the chemical properties of the testing fuel but are also influenced by the local temperature field, fuel distribution, and boundary layers as well as the engine operating conditions [59,60]. For this reason, HCCI combustion using a fuel with an intensive low-temperature reaction exhibits a clear two-stage heat release, whereas fuel with a weak low-temperature reaction exhibits a single-stage heat release. Therefore, this investigation represents an important step towards the goal of achieving clean combustion with high efficiency through the harmonic control of engine operating conditions and

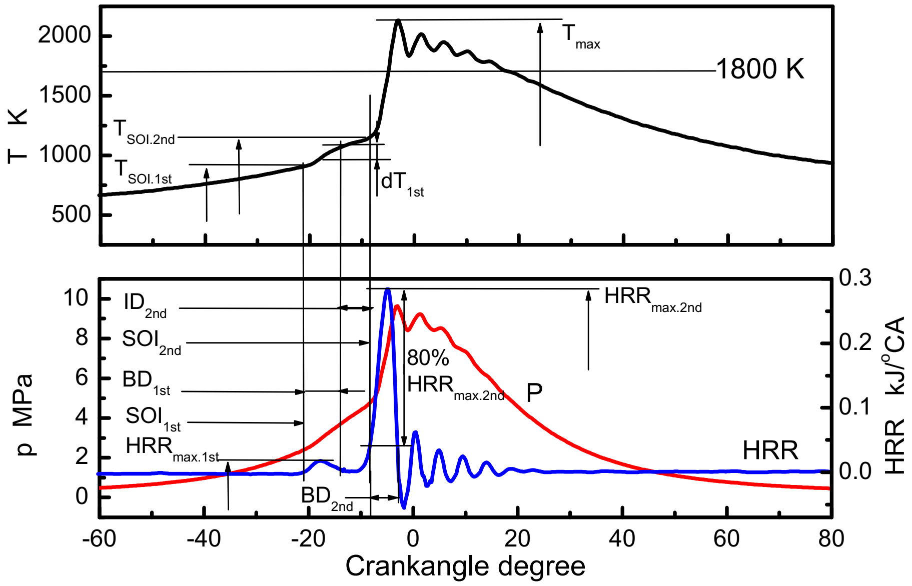

Fig. 1. Classic HCCI combustion characteristics of hydrocarbon fuel [59].

boundary layers, as well as changes in the intermediate elementary reaction rate, reaction pathways, and the concentrations of key species and radicals by fuel design.

2.3. Auto-ignition index for hydrocarbons under HCCI operation conditions

For traditional direct injection compression-ignition engines, the principal parameter used to characterize fuel chemical properties is the cetane number. In the case of SI engines, because of the limitation of knocking combustion, the most important parameter used to characterize fuel chemical properties is octane number. Under HCCI operating conditions, ensuring that self-ignition occurs reliably at the proper time in each cycle regardless of the changing conditions is a challenging task. Previous studies have indicated that the ignition behavior under HCCI conditions cannot be examined by traditional measurements of auto-ignition quality for fuels, such as research octane number (RON) and cetane number. Commonly, the requirements for testing fuels under practical HCCI combustion conditions cover both the ignition quality (cetane number) and anti-knock property (octane number) at both lean and rich-limit conditions. For this reason, traditional cetane or octane numbers may not be optimal parameters for characterization. Another point that should be considered is that the ignition timing, combustion rate, and pollutant emissions may present different behavior for a group of test fuels with the same cetane number or octane number due to the differences in molecular structure and fuel components. Bessonette et al. [61] suggested that the best fuel for HCCI operation may have auto-ignition qualities between those of diesel fuel and gasoline. Using a compression ratio of 12:1 and a fuel with a derived cetane number of 27, they were able to extend the HCCI operating range to 16 bar BMEP. Furthermore, their results showed a low load operation below 2 bar BMEP and required a derived cetane number of 45. Thus, it may be beneficial to explore HCCI operation using fuel blends optimized for specific operating conditions. This also means that the traditional RON and MON numbers are not sufficient indicators of fuel auto-ignition sensitivity when the engine is operated in HCCI combustion mode. Westbrook et al. [62,63] and Silke et al. [64] compared the ignition and combustion rates of nine heptane isomers to clarify the role of molecular structure on the rate of combustion. They found that the same characteristic negative temperature coefficient behavior was observed for each of the isomers, whereas the reactivity and burn durations were different for all isomers.

Koopmans et al. [65] evaluated the influence of octane number on HCCI combustion with negative valve overlap (NVO) technology. Fifteen different fuels with high octane numbers were tested, six of which were primary reference fuels (PRFs) and nine of which were commercial fuels or reference fuels. In these results, no correlation was found between the center point of heat release (CA50) and the research octane number (RON) or motor octane number (MON). However, when only PRFs were considered, a correlation was found between the auto-ignition timing and the RON. Yao et al. evaluated the effects of fuel chemical properties and intake charge pressure on HCCI combustion and found that the effects of PRF octane number on start of combustion were weakened as the boost pressure was increased, and that the PRF octane number had little effect on HC, CO, and NO*x* emissions when supercharging was employed [66]. To define an optimal index to characterize fuel properties under HCCI conditions, some oil companies including Shell Global Solutions, Nippon Oil Corporation, Institut Francis du Pétrole (IFP), and ExxonMobil Research and Engineering [67] have conducted a wide range of research examining the effects of octane number, fuel sensitivity, fuel molecular structure, fuel components, and operating conditions on HCCI auto-ignition quality.

2.3.1. Octane index

In 2003, Kalghatgi et al. proposed the Octane Index (OI) defined in (1) to identify ignition quality under HCCI combustion conditions [68].

$$\mathrm{OI} = (1-\mathrm{K})\mathrm{RON} + \mathrm{KMON} = \mathrm{RON} - \mathrm{KS} \tag{1}$$

Here, K is a constant that depends on the engine-operating conditions and S is the fuel sensitivity. For HCCI operation with PRFs, S is 0. The higher the OI, the more the resistance to auto-ignition and the later the heat release.

Risberg et al. assessed the HCCI auto-ignition quality for 37 operating conditions using fuels with different chemistries and different known RON and MON values [69]. Five categories of fuels were evaluated: paraffinic fuels blended from iso-octane and n-heptane, aromatic fuels blended from toluene and n-heptane, olefinic blends containing di-isobutylene (DIB), n-heptane and iso-octane, and oxygenate blends of ethanol, n-heptane and iso-octane. The fuels were blended so that several fuels had the same RON value but different MON values. The varying MON values were due to the different chemistries of the fuels, the RON values varied between 94.7 and 73, and the sensitivity varied between 11.6 and 0. The results showed that auto-ignition quality is strongly influenced by T_{comp15}, and also, to some extent, by the equivalence ratio, whereas engine speed has little influence. T_{comp15} indicates the temperature at which the pressure reaches 15 bar during the compression stroke. At each operating condition, there is an ideal fuel with $\text{OI} = \text{OI}_0$ such that heat release occurs at top dead center (TDC). OI_0 increases with increasing P_{maxcomp} and T_{maxcomp}, the compression pressure and temperature at TDC, respectively, and decreases with increasing air–fuel ratio and engine speed. For a given RON, sensitive fuels will have auto-ignition qualities close to the requirements of the engine over a wider operating range [70]. However, it is well known that EGR has been widely used to control the ignition and combustion rate of HCCI combustion, but there is no evidence that suggests there are additional effects of EGR on auto-ignition due to changes in the thermodynamic parameters caused by EGR [71].

For practical diesel fuel and gasoline, from the viewpoint of volatility and mixture formation, Kalghatgi et al. suggested that gasoline fuels have an advantage over conventional diesel fuels because they are more volatile [72]. Conventional diesels with an OI less than approximately 35 are also very prone to auto-ignition. With a compression ratio of 14, OI_0 is roughly 50 at low loads and must be much higher at high loads. Thus, it will be much more difficult to attain satisfactory HCCI combustion with diesel fuels unless OI_0 is reduced by reducing the compression ratio. However, the difficulty of self-ignition under low loads could be more easily overcome via control strategies, such as retaining high levels of hot internal EGR or other thermal management strategies. In this respect, it is reasonable to conclude that conventional gasoline fuels are more suitable for a "full HCCI" engine than are conventional diesel fuels. In commonly, they define diesel fuels as those with Cetane Number (CN) > 30 and gasoline fuels as those with CN $< \sim 30$ or Research Octane Number (RON) > 60.

2.3.2. CAI index

Jueland et al. from IFP proposed a CAI Index to characterize the influence of fuel formulation on HCCI combustion. The CAI index was employed to precisely quantify fuel impact on four defined CAI zones, including low speed/low-load, low-speed/high-load, high-speed/high-load, and high-speed/low-load zones [73]. This index is used to compare the operating window in HCCI mode obtained from the selected fuels with that obtained from the reference fuel.

Fig. 2 gives the definition of the CAI index. The surfaces of each load-speed region were calculated for both reference fuel and tested fuels. The CAI index is then defined in each region as the ratio between the two surfaces and is expressed as a percentage. To give more importance to the full-load operation in conventional mode, which erases the improvement allowed in HCCI mode, a modified CAI index was proposed as follows [73]:

$$\text{Mod HCCI index} = \frac{\text{Tested fuel HCCI surface}}{\text{ref fuel HCCI surface}} \bullet \frac{\text{Max power tested fuel}}{\text{Max power ref fuel}} \qquad (2)$$

The authors selected EN228 European specifications as the reference fuel, without oxygenated compounds or additives. HCCI combustion using the reference fuel with the addition of hexane, methanol, ethanol, 2-ethylhexyl nitrate (2-EHN), DMM, and methanol was compared with that of the base fuel. In the low speed/low load zone, a strong impact from 2-EHN blend fuels was observed, and methanol seemed to strengthen this 2-EHN impact. In the high speed/low load zone, strong positive fuel impacts were observed with methanol and 2-EHN blend fuels. In the high-speed/high-load and low-speed/high-load regions, slightly positive fuel impacts were observed for all kinds of additives. These results suggest that the recommended fuel formulation elements for low load enlargement are a cetane improver additive and methanol or ethanol. However, the best fuel formulation element for high load enlargement at low engine speed would be an ethanol blend. With its high latent heat of vaporization, ethanol leads a large "cooling effect" and produces an interestingly high RON value [75]. Table 4 summarizes the effects of physical–chemical properties on each operating region [76,77].

2.3.3. HCCI index

To evaluate the manner in which fuel properties impact HCCI combustion, Shibata et al. conducted an engine experiment using various octane number fuels (RON70, 80, and 92) with the same distillation by blending model fuels chosen from 12 hydrocarbon constituents, as shown in Fig. 3 [78]. The results suggested that RON92 fuel has a small low-temperature heat release and a slow high-temperature heat release. In the case of high engine speed, misfire occurs due to the late high-temperature heat release. Furthermore, the effect of fuel chemical components on LTR was also investigated by comparing the HCCI combustion of the base blend alone, the base blend + 6.5% toluene, and the base blend + 6.5% n-heptane. The heating value and onset crank angle of the LTR differed remarkably for the three fuels and also altered the HTR and HCCI engine performance. Thus, it can be concluded that fuel components selection may be one of the most important factors in HCCI combustion. In general, paraffins exhibited substantial low-temperature reactions, resulting in a larger amount of LTR than olefins, whereas aromatics were very stable at low-temperature ranges and had virtually no LTR. It should be noted that a fuel with a large heating value in the LTR is described as "easy knock, high

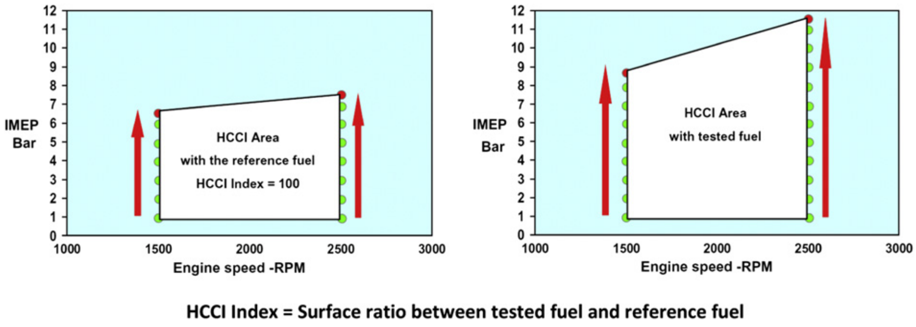

Fig. 2. Definition of CAI index [74].

Table 4
Correlations between HCCI operating regions and fuel properties [76,77].

	Low speed Low load	Low speed High load	High speed High load	High speed Low load
MON	−			−
Cetane index	+	−		+
Heating value	+	−		+
Intermediate boiling point	+	−		+
Final boiling point				
C%	+	−	−	+
H%	+	−		+
O%	−	+	+	−
Low heating value	−	+		−

speed, and low torque", whereas a fuel with a small heating value of LTR presents a "difficult knock, low speed, and high torque". A small change in chemical composition can significantly change the amount and the phasing of LTR and thus affect the HTR [78].

As the amount of low-temperature heat release is primarily dependent on the chemical properties and operating conditions, Shibata et al. further assessed the effects of fuel composition on LTR heating value, LTR CA50, high-temperature heat release, and engine performance for HCCI combustion using 12 different model fuels that were blended from 11 pure hydrocarbons [79]. Due to the substantial LTR heat release of n-hexane, the LTR heating value and LTR CA50 can be altered by changing the n-hexane volume in the blends. From the heat release rate, it was apparent that n-paraffins yield the greatest contribution to a large LTR heat amount, followed by iso-paraffins. Correspondingly, the propensity for early initiation of HTR was clearly distinguishable by fuel group in the order: n-paraffins > iso-paraffins > olefins > naphthens = aromatics.

In general, knocking, combustion, and misfire performance can be described by the parameter HTR CA50. For this reason, Shibata et al. established a correlation between chemical properties and HTR CA50 as follows:

$$\begin{aligned}\text{HTR}\quad \text{CA50} &= A \bullet (n - Ptan\,e\ \text{vol\%}) \\ &= +B \bullet (\text{Cyclopen tan}\,e\ \text{vol\%}) + J \bullet (\text{Toluene vol\%}) \\ &\quad + K \bullet (m - \text{Xylene vol\%})\end{aligned} \tag{3}$$

$$\text{HTR}\quad \text{CA50} = \text{G(LTR CA50,}\quad \text{LTR heating value)} \tag{4}$$

This function can be used to evaluate the fuel component contribution towards the advancement of the phase of HTR. Accordingly, an HCCI index was proposed for considering the correlation of fuel components and HTR CA50 as follows [80]:

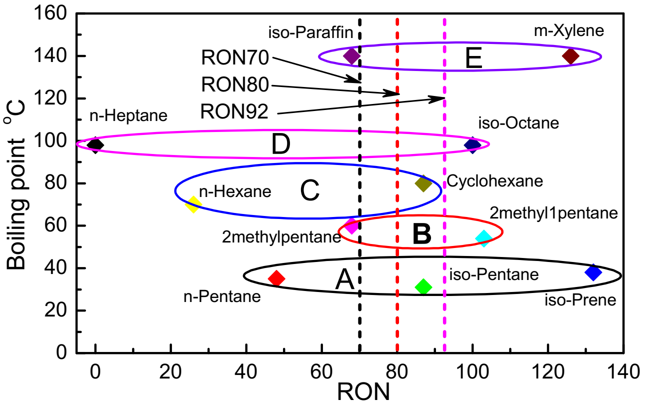

Fig. 3. Boiling point-RON map of the fuel components [78].

$$\begin{aligned}\text{HCCI}_{\text{index}} &= m \bullet \text{MON} + \text{a} \bullet (\text{n} - \text{P}) + \text{b} \bullet (\text{i} - \text{P}) + \text{c} \bullet (\text{O}) \\ &\quad + \text{d} \bullet (\text{A}) + \text{e} \bullet (\text{OX}) + \text{Y}\end{aligned} \tag{5}$$

where MON indicates motor octane number, n-P denotes the n-Paraffins vol%, i-P is the iso-Paraffins vol%, O is the Olefins vol%, and A is the Aromatics vol%. A smaller HCCI index demonstrates an increased ignitability, as is usually the case with octane numbers. Fig. 4 displays the absolute auto-ignition characteristics for different hydrocarbon fuels.

2.4. Fuel design strategies and methods for HCCI combustion

It is widely accepted that HCCI combustion is essentially dominated by the chemical kinetics of fuel/air mixtures under practical engine operating conditions. Fuel physical–chemical properties, as well as spatial and time histories, have dominant effects on ignition and combustion. Furthermore, a large number of studies have shown that traditional commercial fuels or sole-component fuels cannot meet the requirements for HCCI combustion. For these reasons, it is necessary to reform or design the molecular structure of fuel, fuel components and composition, and physical–chemical properties to make them more suitable for practical engine combustion. The principles of this concept are shown in Fig. 5.

(1) Cetane number: A high cetane number has the significant potential to promote cold starting, broaden the lean-burn limit, reduce cycle-to-cycle variation, improve mode transition characteristics, and depress HC and CO emissions, but it has a negative effect on the rich-burn limit.
(2) Octane number: Octane number has an effect almost opposite to that of the cetane number.
(3) Molecular structure: Paraffins have only LTHR-enhancing characteristics, aromatics have only LTHR-inhibiting effects, olefins and naphthenes have both LTHR-enhancing and -inhibiting effects, and the difference between the LTHR-enhancing and -inhibiting effects is noticeable.
(4) Oxygen content: This factor has a positive effect that broadens the load limit and improves the local combustion efficiency and emissions.
(5) Latent heat of evaporation (LHE): A large LHE is favorable to the depression of the initial temperature at the beginning of the compression stroke, delay of the ignition timing, reduction of the maximum combustion temperature, and partial elimination of knocking combustion.
(6) Boiling point and distillation: A lower boiling point and distillation temperature improves the potential to form homogenous mixtures, eliminates the local fuel zone, reduces the maximum combustion temperature, and reduces the NO*x* and PM emissions.

The precise control of ignition timing, the proper combustion rate and center crank angle, the avoidance of knock, and the preservation of combustion completion are key aspects of HCCI combustion. Thus, it is necessary to reconfigure fuel properties and compositions to improve the adaptability and compatibility of different fuels for HCCI combustion under a wide operating range. Fuel additives, fuel blending, dual-fuel technology, and optimized fuel proportion in real-time can all be used to redesign the chemical properties of the in-cylinder mixtures. Indeed, the fuel design concept was first proposed by Senda et al. [81,82] and was used to improve the combustion and emissions for a traditional DICI engine. Recently, this concept has been more widely used to control and optimize advanced combustion modes.

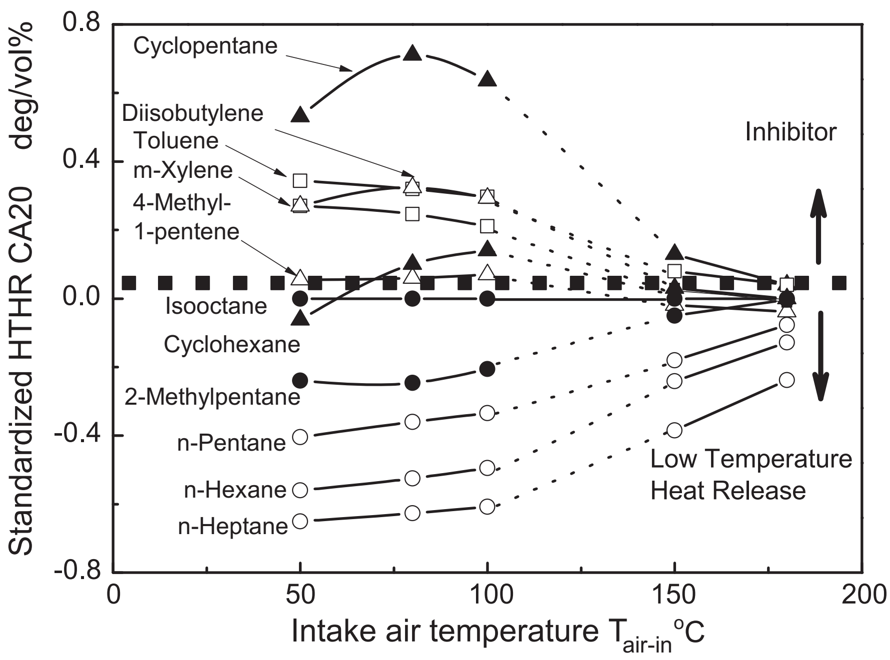

Fig. 4. Absolute auto-ignition characteristics of hydrocarbons [80].

3. Fuel design for the control of HCCI combustion

3.1. Fuel design for PRFs HCCI combustion

In general, high cetane number fuels feature favorable flame ignitability, and therefore, they tend to extend the lean-burn area for HCCI combustion. At the same time, excessively early ignition timing and excessively fast combustion rates under richer fuel/air mixtures lead to knocking combustion, which limits the engine's operation ranges. Thus, HCCI combustion with high cetane number fuels faces obstacles at larger loads. However, HCCI combustion with high octane number fuels is favorable for operation at richer fuel/air mixtures, with ignition timing showing a strong sensitivity to mixture concentration and temperature. In particular, misfire or partial burn may be observed under lower engine load, lower initial temperature, and mode transitions. Thus, the important challenges in HCCI combustion with high octane number fuels are cold start and lean-burn regions.

3.1.1. Inert additives for HCCI combustion with high cetane number fuels

For high cetane number fuels, previous studies have revealed that their oxidization process under low-temperature ranges consists mainly of H atom abstraction from the fuel, oxygen addition, isomerization reactions, and the decomposition of the keto-hydroperoxide molecule. The chain-branching reactions produce a large number of OH and other active radicals, thus triggering a cool-flame reaction at a certain temperature. This occurs precisely because of the exothermic reaction of LTR and the large amount of H_2O_2 that accumulates in the NTC region, leading to excessively early ignition and knock tendencies for richer fuel/air mixtures [83]. To delay the ignition and combustion phasing, an inert additive may be used to alter the reaction pathways, depress the OH formation reaction or strengthen the OH consumption reaction, and reduce the heat release in low-temperature ranges.

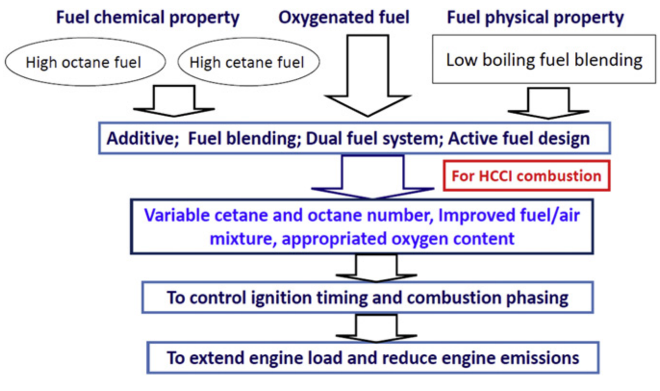

Fig. 5. Fundamental principles of fuel design for HCCI combustion.

Hashimoto et al. confirmed the inhibiting effects of ethanol on HCCI combustion of n-heptane using an RCM under various conditions [84]. The experimental results also indicated that ethanol effectively retarded the hot ignition period of HCCI combustion due to its effective retardation of the cool-flame period. Saisirirat et al. [85] compared the ignition phasing of LTR and HTR for ethanol/n-heptane, n-butanol/n-heptane, and iso-octane/n-heptane blends. The results showed that increasing the ethanol, n-butanol, or iso-octane fractions reduces the percentage of LTHR combustion and moderately increases that of the IMEP. Moreover, the addition of both alcohols to n-heptane has a larger impact on delaying the heat release rate than that of iso-octane when the blended RON, MON, and CN are considered. Motivated by the need for the precise control of auto-ignition during the compression stroke of HCCI combustion, Subramanian et al. [86] numerically simulated the chemical influence of CO and H_2 additions on the auto-ignition of n-heptane/air mixtures. The simulated results further validated the hypothesis that the presence of CO at low temperatures ($T = 600$ K) lengthens the delay by approximately 5%–10%, whereas at high temperatures ($T = 1000$ K), it shortens the delay on the order of 15%–20%. H_2 addition at low temperatures significantly lengthens the delay; at high temperatures (1000 K), this modification does not considerably influence the delay, although this depends on the added amount.

Lu et al. compared the inhibition effectiveness of n-heptane HCCI combustion with various additives, including methanol, ethanol, isopropanol, and MTBE [87–90]. From the point of view of their anti-

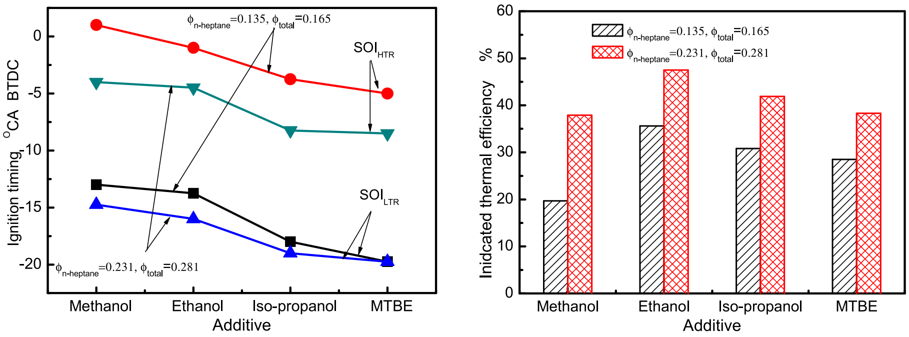

Fig. 6. Comparison of the effects of additives on n-heptane HCCI combustion [87].

knock effects, the octane number increases in the order MTBE < iso-propanol < ethanol < methanol, thus the suppression effectiveness of the four additives increased in the order MTBE < iso-propanol << ethanol < methanol. This may be attributed to the lower activation energy barrier of the H atom abstraction by H, CH3, and OH as well as other radicals from the high-carbon alcohols and a high activation energy barrier for low-carbon alcohols. Due to the stronger depression effect of the methanol additive on the low-temperature reaction, n-heptane HCCI combustion with a methanol additive exhibits very late ignition timing and combustion phasing, which lowers the thermal efficiency, as seen in Fig. 6. Meanwhile, the moderate depressive effect of ethanol on the n-heptane HCCI combustion produced proper combustion phasing and optimal thermal efficiency.

3.1.2. *Active additives for HCCI combustion with high octane number fuels*

High octane number fuels such as iso-octane and toluene feature a longer ignition delay due to the weak and slow LTR [91,92]. To precisely control the self-ignition of gasoline-like fuels near TDC, additional methods—including internal exhaust gas recirculation (EGR), variable compression ratio (VCR), and variable valve timing (VVT)—can be used to change the effective compression ratio and/or the amount of hot exhaust gases retained in the cylinder as necessary. Additionally, by adding an active additive to the base fuel, the proper thermal atmosphere environment can be created in the core areas of the combustion chamber due to the heat release and active radicals produced by additive oxidation during the compression process. As a result, the ignition chemistry timescale is shortened, the combustion rate is enhanced, and combustion stability and thermal efficiency under lean-burn conditions are promoted [93]. Fig. 7 illustrates that a minor addition of additive has the ability to trigger HCCI combustion using PRF90 without any additional methods.

Peroxides such as H_2O_2, 2-EHN, and DTBP are common fuel additives. In particular, DTBP dissociates at intermediate temperatures to produce two tert-butoxy radicals $(CH_3)_3O$ that quickly dissociate to form acetone and methyl radicals. Acetone is a stable species below 900 K and cannot contribute to the improvement of combustion characteristics, whereas the methyl radical is reactive and forms products such as formaldehyde, methanol, and hydrogen peroxide that enhance hot ignition. DTBP also significantly increases the reactivity of neat iso-octane. The addition of 1% DTBP doubles the peak CO concentration and increases the temperature range of the low-temperature reaction regime from 60 K to 150 K [95,96]. With the addition of a small volume of DTBP, the ignition delay, the cycle-to-cycle variations, and the stable operating ranges were improved [97]. As an example, Eng et al. confirmed that the HCCI light-load combustion stability limit was broadened from a fueling rate of 9 mg/cycle with neat gasoline to 6.2 mg/cycle with a 15% DTBP addition [98].

3.1.3. *HCCI combustion characteristics of PRFs and their mixtures*

Other than the addition of additive to high cetane number or high octane number fuels, the most effective way to improve fuel adaptability is to blend two fuels with opposite chemical properties. Fig. 8 provides a comparison of the combustion characteristics of PRFs and their mixtures under the same equivalence ratio. It can be seen from the figure that both the LTR and HTR of n-heptane HCCI combustion occurred very early, whereas with the increase of the iso-octane volume, equivalent to the increase of the octane number, the combustion phasing of the LTR and HTR was gradually delayed. Two-stage heat release was observed, but the LTR weakened gradually with the RON range variation from 0 to 75. As a result, the maximum heat releases of PRF50 and PRF75 HCCI combustion were concentrated near to the TDC. Another point that can be inferred from this figure is that the main heat release sometimes occurs during the compression stroke, due to the

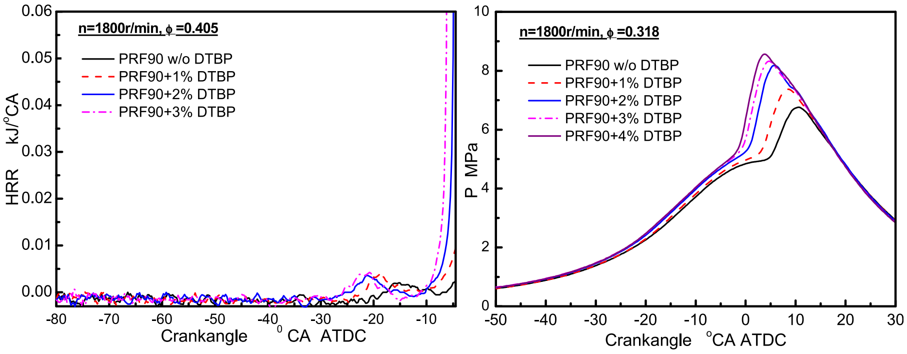

Fig. 7. Effect of additive addition on PRF90 HCCI combustion [94].

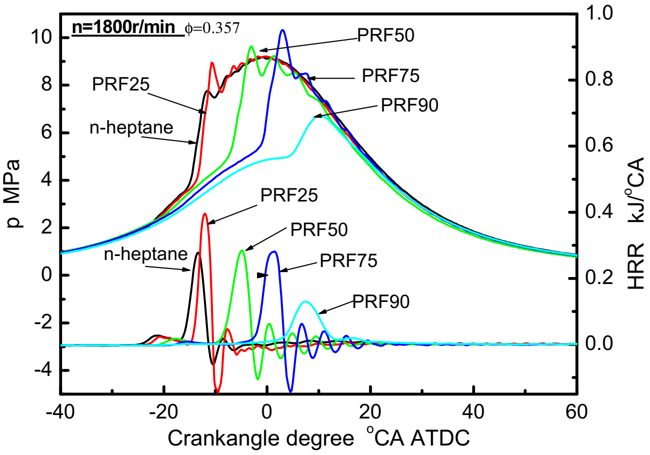

Fig. 8. Comparison of HCCI combustion characteristics with different PRF mixtures [59,60].

excessively earlier combustion phasing, and on other occasions can occur during the expansion stroke for the excessive late combustion phasing. These two types of combustion events negatively affect thermal efficiency and load expansion because of negative piston work or larger heat losses, respectively. In this figure, it should be noted that HCCI combustion with PRF90 operated stably only if the coolant temperature was higher than 92 °C when the inlet temperature remained at 20 °C. Additionally, the combustion quality and emissions deteriorate with decreases in the equivalence ratio, inlet charge temperature, and coolant temperature.

Fig. 9 shows the effect on the amount of heat release of n-heptane volume in PRF mixtures during the LTR, ignition timing of the LTR, and correlation between the combustion phasing of the LTR and HTR. It is apparent that the cumulative heat release decreases linearly with the increase in fuel octane number. From this, it can be deduced that the heat release during the first stage is largely dependent on the mole concentration of the high cetane number fuel (such as n-heptane in this section). The start of the LTR is postponed significantly with the increase in fuel octane number, but is slightly advanced with increases in the equivalence ratio. For a specific fuel test, the second-stage ignition timing is almost linear with the first-stage ignition timing.

As stated above, for HCCI combustion with PRFs and their mixtures, the overall ignition delay is mainly correlated to the n-heptane/oxygen mole ratio but is less sensitive to the iso-octane to oxygen ratio [99]. The induction time between the LTR and HTR depends primarily on the amount of heat release during the LTR. In addition, higher intake charge pressure and lower initial temperature will produce a larger heat release during the LTR, whereas the charge temperature at the end of the LTR has nothing to do with the intake air temperature. For this reason, HCCI combustion phasing using PRFs and their mixtures can be modulated by n-heptane mole concentrations.

The HCCI combustion operating load with PRFs and their mixtures is limited by the maximum pressure-rise rate or ringing intensity, the acceptable NO*x* emissions level, cycle-to-cycle variations or operating stability, tolerable levels of HC and CO emissions, and engine configuration parameters such as the compression ratio, engine speed, and combustion chamber geometry. Sjoberg et al. explored the high load limits of HCCI combustion using iso-octane, PRF80, and PRF60 under naturally aspirated operation conditions. The experimental results show that the actual load-limiting factor is dependent on the auto-ignition reactivity of the fuel, the selected CA50, and, in some cases, the tolerable level of NO*x* emissions [100]. For low-reactivity fuels, such as iso-octane, which has the highest resistance to auto-ignition, unacceptable NO*x* emissions limited the maximum IMEP due to the high intake temperature requirement. For a very reactive fuel, large amounts of EGR, which are required to control the combustion phasing, limited the maximum IMEP. A fuel of intermediate reactivity, PRF80, exhibited the highest IMEP.

3.1.4. HCCI combustion characteristics of TRFs and their mixtures

Practical distillate fuels such as gasoline or diesel are composed of many classes of hydrocarbons, including alkanes, isoalkanes, alkenes, cycloalkanes, and aromatics, among others, and this creates intolerable complexities in the chemical kinetics. In this case, it is useful to employ the idea of a surrogate fuel, or a model fuel that describes the behavior of combustion of real fuels with several representative components of each class of hydrocarbon. In addition to n-heptane and iso-octane, toluene is often used as one component of gasoline surrogate fuels [101]. To accurately simulate the ignition properties and chemical kinetics of practical fuels, linear alkanes (n-heptane), branched alkanes (iso-octane), and aromatics (toluene) were selected and blended as the base testing fuel, toluene reference fuel (TRF) [102,103]. With regards to the PRFs and TRFs, the ignition delay shows significant differences even at the same octane number. At lower intake charge temperature and high boosting pressure, TRFs exhibit a strong anti-knock combustion ability, whereas under the lower intake charge pressure and higher initial temperature conditions, they show similar ignition phasing [104].

The engine experimental results showed that the hot ignition temperature of toluene is about 200 °C higher than that of common hydrocarbons. As a result, the HTHR combustion period of n-heptane/toluene blend fuels was longer than that of the other fuels because of dual-phase high-temperature heat release (DP-HTHR) combustion, as shown in Fig. 10. The first part of the HTHR is caused by n-heptane, and the second is caused by benzyl radicals and aromatics produced from toluene. The most important and most interesting finding is the

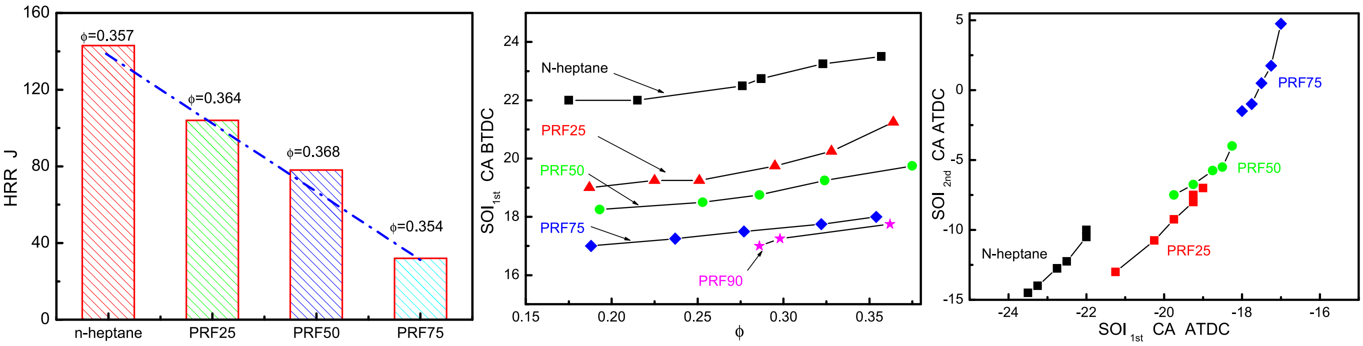

Fig. 9. The effects of n-heptane volume on heat release amount and ignition timing of the LTR and the relationship between the onsets of LTR and HTR [59,60].

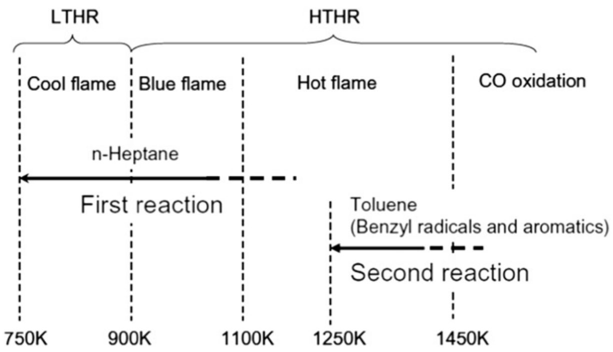

Fig. 10. Heat release mode and ignition mechanism of DP-HTR combustion [104,105].

existence of the second-peak heat release, as the DP-HTHR has the potential to extend the engine operational range to high-load conditions and reduce engine combustion noise. To prove that the second HTHR of the DP-HTHR was not caused by a rapid CO oxidation process but by the decomposition and oxidation of the benzene ring in toluene (benzyl radicals and aromatics), the exhaust emissions and combustion characteristics were analyzed with the same HTHR CA50 and IMEP conditions using DP-HTHR fuel and other fuels [105]. The results confirmed that the decomposition and oxidation of the benzene ring at the hot flame temperature was the starting trigger for the second HTHR in DP-HTHR combustion. Therefore, the IMEP of n-heptane/toluene blends was 30% higher, and the coefficient of variation (COV) was the lowest of the other fuels [106,107], as can be seen in Fig. 11. The key problem of DP-HTHR combustion is to find a group of fuels with different hot ignition temperatures. There are many fuel variations that are able to achieve DP-HTHR combustion with a combination of high- and low-reactivity hydrocarbons. The n-paraffin families represent the highly reactive hydrocarbons, and aromatic families have a lower reactivity. Multi-phase HTHR (MP-HTHR) combustion can also be achieved by an appropriate choice of hydrocarbons.

3.2. Alternative fuels HCCI combustion

It is well known that fuel diversification is generally required for the future generation of internal combustion engines. Other than natural gas or compressed natural gas (CNG), which have been widely used as commercial fuels in an extensive range of applications, other renewable fuels such as ethanol and methanol have also been used as partial substitutes for gasoline fuel. In addition, some preliminary investigations have attempted to utilize dimethyl ether and butanol as alternative engine fuels.

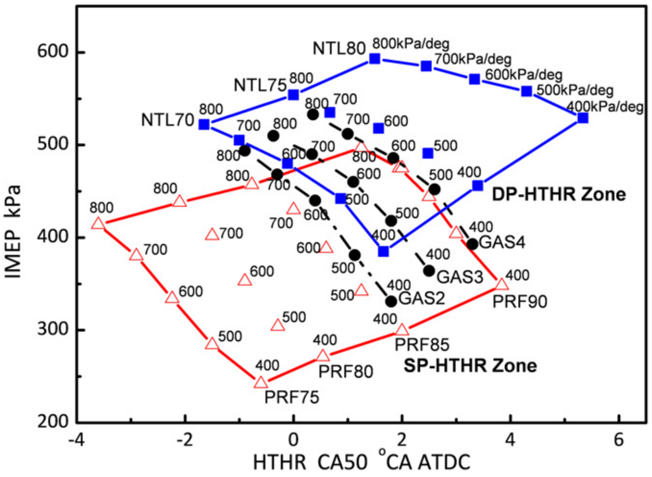

Fig. 11. Load expansion capacity of DP-HTR combustion [105].

3.2.1. Natural gas

Natural gas or CNG consists of methane, ethane, propane, butane, pentane, hexane, and many other minor gas constituents, and its composition can also vary with the source of the gas. Although almost all of these alkanes are straight-chain rather than branched-chain, a stronger carbon bond gives them a tendency not to react with oxygen at low to medium temperature ranges. Therefore, the required initial temperature for CNG HCCI combustion means that the fuel should be preheated to a higher level. In the early stage, CNG HCCI combustion is always achieved by intake charge preheating or an enhanced compression ratio [108,109]. To clarify the influence of butane on the self-ignition and combustion of CNG, Jun et al. preheated the intake air using an electric heater installed in the intake manifold [110]. A butane tank was used to change the fuel components of the CNG. Experimental results showed that the CNG auto-ignition temperature varied over in range of 900–1100 K for different butane percentages, but the simulated results predicted auto-ignition at approximately 1072 ± 22 K regardless of the equivalence ratio, intake temperature, intake pressure, external EGR rate, and engine speed [111]. Yanmar Co., Ltd. and the University of Shiga Prefecture proposed a CNG HCCI combustion method that is similar to that of gasoline HCCI combustion based upon exhaust gas rebreathing technology. The intake valve, together with the exhaust valve, is opened slightly at the beginning of the exhaust stroke. In this way, part of the burned gas, which is at high temperature, is introduced backwards into the intake pipe, resulting in an increase in the intake-gas temperature [112]. In this manner, CNG HCCI combustion was achieved with proper compression ratio, coolant preheating, and spark-assisted technology without the use of additional electrical preheating technology [113].

Fuel composition, particularly the elevated hydrocarbons content (ethane, propane, and butane) of the fuel is of primary concern. Fuel composition influences HCCI operation both in terms of design, via compression ratio and initial charge temperature, and also in terms of engine control. To achieve CNG HCCI combustion, complex technologies such as intake preheating, enhanced compression ratio, and internal exhaust gas recirculation by modulation of the valve train will lead to modification of the engine configuration. In addition, the mode transitions between SI/HCCI/SI are relatively troublesome to implement in the control strategy. For these reasons, a compound HCCI combustion method that features a pilot injection of diesel fuel to ignite a homogenous CNG/air mixture is an effective method for achieving improved combustion efficiency and higher indicated thermal efficiency [114]. In 2001, Stanglmaier et al. demonstrated CNG HCCI combustion, assisted by Fisher-Tropsch (F-T) naphtha as a secondary fuel, in the idle-up load regime up to 35% of the peak torque; however, this work used conventional spark-ignited natural gas combustion for the high-load regime. Using this dual-fuel and dual-mode combustion approach, the maximum power output and high-load fuel efficiency was unchanged from those of the base engine, but yielded a 10–15% improvement in the low-to-moderate-load fuel efficiency. In addition, engine-out NO*x* emissions during HCCI operation were over 90% lower than that of spark-ignited natural gas operation over the equivalent load range [115]. Gong et al. injected a small pilot quantity of diesel fuel during the compression stroke to improve the HCCI power output. The simulated results showed that the required initial temperature for ignition was reduced by about 70 K for the cases with the diesel pilot charge, and a 25–35% increase in power density was achieved without adverse impacts on the NO*x* emissions [116]. In another example, pilot injection of n-heptane accompanied by intake charge preheating and external

EGR was used to extend the CNG HCCI operating ranges by Handford et al. [117].

It has been demonstrated that the CNG composition has a significant effect on ignition because greater concentrations of higher hydrocarbons tend to significantly lower the ignition temperature of the mixture [118]. Additionally, it has been confirmed that CNG ignites when the in-cylinder temperature reaches 1000 ± 100 K [119]. Then, active control strategies can be used to compensate for possible changes in composition, including the use of an ignition promoter additive [120]. Mohammadi et al. investigated the effects of ozone intake addition on the performance and emissions of a naturally aspirated single-cylinder PCCI natural gas engine under different equivalence ratios and with variable amounts of ozone addition [121]. The results indicated that ozone effectively enhances the ignition of natural gas and improves the thermal efficiency and emissions of THC and CO, especially under low engine loads. Rough estimation indicates that an addition of 100 ppm of ozone to the intake-gas corresponds to a 40 °C increase in the intake air temperature. CNG auto-ignition with ozone addition becomes feasible by generating OH via H_2O_2. The influence of ozone addition on ignition angle is roughly the same as that of direct injection of an oxygen radical, and this addition is one order of magnitude more effective than the addition of an OH radical [122]. HCCI combustion at low loads often suffers from excessive cyclic variations because the homogeneous charge is too fuel-lean to burn completely. If natural gas is used, these variations can be further exacerbated due to the relatively narrow operational limits of methane. However, Wong et al. confirmed that the addition of hydrogen, which has a relatively wide operating range, to CNG can reduce cyclic variations while extending the operating region of the HCCI combustion [123]. Morsy et al. compared the effect of additives such as dimethyl ether (DME), formaldehyde (CH_2O), and hydrogen peroxide (H_2O_2) for ignition control in natural gas HCCI engines [124,125]. At a fixed equivalence ratio of 0.3 and an initial mixture pressure of 1.5 bar, it was observed that an additive-free mixture did not ignite for an intake temperature of 400 K. A mixture containing a small quantity of additives at the same temperature, however, was successfully ignited. For a fixed quantity of additive, it was found that H_2O_2 addition was more effective in advancing the ignition timing as compared to the other two additives. Furthermore, the addition of even 7 vol% of H_2O_2 could ignite the mixture at an intake temperature of 350 K, whereas fractions of at least 12.5 vol% and 35 vol% were needed for DME and CH_2O, respectively. Noorpoor et al. conducted a similar study to evaluate the effect of additives such as hydrogen (H_2), hydrogen peroxide (H_2O_2), formaldehyde (CH_2O), and ethane (C_2H_6) on natural gas HCCI combustion [126]. Furthermore, reformer gas, which contains a large proportion of CO and H_2 [127,128], and cetane number improver of DTBP [129], have the capability to improve CNG auto-ignition under HCCI conditions.

3.2.2. *Dimethyl ether*

DME appears to be an excellent and efficient alternative fuel for use in diesel engines and produces almost smoke-free combustion. This is not only because of its low auto-ignition temperature and its almost instantaneous vaporization when injected into the cylinder, but also because of its high oxygen content (approximately 34.8% by mass) and the absence of C–C bond in its molecular structure. In addition to smoke-free exhaust, a DME engine yields excellent drivability at lower engine speeds and comparable or improved thermal efficiency and NO*x* emissions [130–134]. Furthermore, DME can be produced from a variety of feed-stocks such as natural gas, crude oil, residual oil, coal, waste products, and biomass. Therefore, it is very attractive in applications for traditional compression-ignition engines.

Furthermore, the physical–chemical properties of DME have made it very attractive for HCCI combustion. According to chemical kinetics, the initial reaction of the DME oxidization process is an unimolecular fuel decomposition that acts to establish the radical pool. After that, H atom abstraction from the fuel becomes more important and forms methoxy-methyl. Methoxy-methyl radicals can undergo two different reactions: addition to molecular oxygen to produce methoxy methyl-peroxy radicals, or B-scission to yield formaldehyde and methyl radicals. Addition to O_2 occurs primarily at low temperatures, as the bimolecular addition of a methoxy-methyl radical to O_2 has no activation energy barrier. Then, the most important reaction step for the methoxy methyl-peroxy radical is isomerization, and then oxygen addition for a second time followed by isomerization to form ketohydroperoxide. The decomposition of the ketohydroperoxide molecule leads to chain branching, as two radicals are formed from its decomposition [135,136]. In low-temperature ranges, chain-branching reactions can trigger the LTR or cool-flame reaction. As the temperature increases through the negative temperature coefficient region, the chain-propagation reactions of alkylhydroperoxide species increase in importance, leading to the formation and decomposition of products, whereas the proportion of chain-branching reactions decreases. Compared to that of other diesel-like fuels, the DME oxidation process features a lower initial temperature and stronger reaction intensity at low-temperature ranges. The significantly earlier and stronger LTR has a negative effect on DME HCCI combustion due to its effects on knock combustion and negative work of the piston [137]. Based on this, the major goal of DME HCCI combustion is to broaden the load limit by optimizing the compression ratio, EGR strategy, valve train actuation, and fuel design method. In other words, the main challenges for DME HCCI engines involve structuring the systems to control combustion phasing, optimizing crank angle at 50% heat release (CA50), retaining high thermal efficiency, and avoiding an excessive rate of pressure rise that causes knocking behavior when operating conditions vary.

Ohmura et al. constructed a two-stage exhaust cam system to introduce hot (internal) EGR gas [138]. By reopening the exhaust valve during the inlet stroke, a part of the exhaust gas can be returned from the exhaust port into the combustion chamber as hot EGR gas. Then, the gas temperature at IVC is controlled by changing the mixing ratio of hot (internal) EGR gas and cold (external) EGR gas. Jang et al. controlled the IEGR rate by changing the intake and exhaust maximum opening points (MOP) as well as the exhaust cam lifts to modulate the combustion phasing and smooth the heat release [139]. In addition, the integration of a port fuel injection combining direct in-cylinder injection, flexible fuel injection timing, and external EGR is the most effective method with which to optimize combustion phasing and broaden the operating ranges [140].

Ogawa et al. attempted to depress excessively early combustion phasing and rapid combustion through the in-cylinder injection of various ignition suppressors, including water, methanol, ethanol, 1-propanol, hydrogen, and methane, so as to expand the operating range in an HCCI engine with induced DME as the main fuel [141]. The reaction suppressors reduced the rate of low-temperature oxidation and consequently delayed the onset of high-temperature oxidation. From the results of numerical simulation and chemical analysis, the depression can be attributed to the reduction of OH radicals. In particular, alcohols had a greater impact on OH radical reduction, resulting in stronger ignition suppression. Yamada et al. confirmed that methanol retarded ignition timing by up to 15 crank angle (CA) with an 8% addition of DME [142]. The associated reduction of cool-flame heat release was the main cause of the final thermal ignition delay. A simple formulation accounting for the retardation effect was established, in which HCHO + OH and methanol + OH reactions are responsible for the termination of the DME chain reaction system in low-temperature oxidation. In contrast, ozone addition advanced the ignition timing up to 20 CA with an estimated addition of only 0.015% of DME. This acceleration is caused by an increase of heat release in the cool flame.

Numerous research efforts have suggested that even if variable valve technology, controllable EGR, variable compression ratio, inhibitor fuel additives, fuel blending, and other techniques are integrated into a single test engine, the dimethyl ether HCCI combustion range would still be very difficult to expand to full engine load condition. Based on ignitability and gas-phase under common environmental conditions, dual-fuel technologies such as DME/CNG, DME/LPG, and DME/methanol and real-time fuel design may be used to control the ignition timing, the center point of heat release, and burn duration. Using these approaches, high efficiency with clean combustion can be produced over wider operating ranges. These points will be discussed in Section 4.

3.2.3. *Hydrogen*

The limited availability of fossil fuel resources, CO_2 issues, and statutory emission regulations have raised the question of how conventional fuels can be replaced by alternative fuels such as hydrogen. Although present research is primarily devoted to developing a hydrogen fuel-cell power plant, other studies have also found that hydrogen is an ideal fuel for internal combustion engines. The development and exploitation of hydrogen engines are based on the consensus that as some countries work toward developing a hydrogen economy, intermediate technologies will be needed to bridge the gap between today's traditional internal combustion engine vehicles and the ultimate goal of hydrogen-powered fuel-cell vehicles. These movements have identified hydrogen-powered internal combustion engine (ICE) vehicles as an important intermediate technology on the path to a hydrogen economy. The second reason for the attractiveness of the hydrogen ICE is that it can be manufactured more cheaply than fuel cells, at a cost that is only about 15% more than conventional gasoline engines [143]. The third attractive feature is the fuel flexibility of ICEs, in that not only pure hydrogen but also hydrogen-enriched gases (or blends), including reformer gas, pyrolysis gas, and marsh gas, can be directly used in an engine with minor modifications. This approach can be used to address the widespread lack of hydrogen fuel infrastructure in the near term. Another benefit of hydrogen engines is that they are CO-, HC-, soot-, and CO2-free, as they only emit NO*x*. Furthermore, hydrogen-powered ICEs also have many operating advantages. They perform well under all weather conditions, require no warm-up, have no cold start issues (even at subzero temperatures), and are highly fuel efficient, up to 25% better than conventional spark-ignition engines [143,144].

As an alternative fuel for ICEs, hydrogen features a higher self-ignition temperature and adiabatic flame temperature, wider flammability limits, a low energy requirement for ignition in air, rapid flame propagation speed, and higher caloric value, among others. Because of these properties, hydrogen in vapor form significantly improves engine operation and life cycle as compared to gasoline. From the viewpoint of engine performance parameters, operation with hydrogen reduces the brake-specific fuel consumption. As a motor fuel, hydrogen is easily ignited by a spark plug with minimal energy, producing a controlled gentle combustion rate under a low compression ratio. For hydrogen HCCI combustion, a necessary compensatory strategy is to increase the compression ratio or enhance the initial temperature of the mixture. At the same time, the combustion rate of a stoichiometric hydrogen/air mixture under the above conditions will increase to an unacceptable speed and ultimately generate an extremely high combustion knock. Thus, a key goal in the development of hydrogen HCCI combustion is to depress the high combustion rate by EGR or leaning of the combustible mixture to reduce the knock effect.

Hydrogen HCCI combustion suffers from unstable run behavior and cycle-to-cycle variations, difficulty in achieving accurate control of ignition timing, and ease of ignition by in-cylinder hot spots located on the engine head and the piston surface. In addition, the start of combustion occurs too early to generate the maximum break torque because both 50% MFB and in-cylinder peak pressure are located before the TDC position of the piston [145]. In addition to higher compression, intake charge preheating is an effective way to promote hydrogen auto-ignition. Meanwhile, an accurate and spontaneous ignition control strategy is necessary with this method. Antunes et al. experimented with hydrogen HCCI combustion with an excess air ratio of six, and a maximum fuel efficiency of 45% was achieved with an excess air ratio of three [146]. However, the maximum power of the engine in HCCI mode is quite modest and is limited by the need for inlet air heating to ensure auto-ignition. Rosati et al conducted an optical investigation of hydrogen HCCI combustion in a single-cylinder research engine equipped with both port fuel injection and direct injection (DI) systems running at 1000 rpm [147]. In this study, HCCI combustion of hydrogen was initially enabled by means of a pilot port injection of n-heptane preceding the main direct injection of hydrogen, along with intake air preheating. Sole hydrogen fuelling HCCI was finally achieved and made sustainable.

Due to the difficulty in experimental study of hydrogen HCCI combustion, numerical studies are often used to optimize the control strategies and engine parameters [148]. Komninos et al. examined the effects of various operating variables on hydrogen HCCI combustion using a multi-zone model [149]. The model takes into account heat transfer between the zones and the combustion chamber walls, providing a spatial temperature distribution during the closed part of the engine cycle. Liu et al. found that an increase in the initial flow swirl ratio or speed lengthens the delay period for auto-ignition and extends the combustion period while reducing NO*x* emissions [150]. Optimum values of the initial swirl ratio and engine speed exist for each mixture intake temperature, pressure, compression, and equivalence ratio in order to achieve high thermal efficiencies and low NO*x* emissions while reducing the knock tendency. It is worth noting that hydrogen is often used as an ignition promoter for CNG and other fuels but not for neat fuels due to the significant difficulty associated with accurate ignition control.

3.2.4. *Alcohols*

Alcohols are promising alternative fuels in vehicle engines due to multiple renewable sources. Ethanol has been widely used as a main fuel, particularly in Brazil, and as a gasoline additive octane improver for improved combustion in the USA and Canada. Although a small amount of ethanol substituted in gasoline has the potential to improve combustion and emissions to a certain degree, the thermal efficiency is not significantly changed. A large number of researchers have attempted to improve the ethanol-fueled engine's thermal efficiency up to diesel-like levels by implementing next-generation combustion modes. To achieve ethanol HCCI combustion, it is necessary to enhance the initial temperature significantly before the end of the compression stroke due to the large latent heat of evaporation and higher octane number [151]. For this purpose, with the application of a valve timing strategy for the inlet and exhaust valves, ethanol HCCI combustion was achieved by varying the amount of trapped residuals through negative valve overlap [152]. Correspondingly, intake charge preheating, a higher compression ratio, and exhaust gas re-breathing can also be used to assist ethanol HCCI combustion. Although the NO*x* emissions were low, the load range was unacceptably small for naturally aspirated HCCI operation with residual gas trapping on a spark-ignition engine. When inlet manifold pressurization was employed, a substantial increase in the upper load boundary could be achieved without any substantial increase in NO*x* emissions [153]. Although the maximum pressure-rise rate increased to a high value with the higher boost pressure [154], it could be depressed by direct injection of water [155]. Furthermore, by the addition of a volume of diethyl ether (DEE) to the ethanol, DEE led the combustion and proceeded further toward overall completion [156]. Xie et al. compared the HCCI combustion behavior of gasoline, E50 (50% gasoline, 50% ethanol), E100 (100% ethanol), M50 (50% gasoline, 50% methanol), and M100 (100% methanol). It was found that the ignition timing of M100 is advanced much more than other fuels, and alcohols have better adaptive capabilities for lean combustion than does gasoline within the attainable HCCI operation range [157].

3.2.5. *Other alternative fuels*

A variety of practical or potential fuels can be used in HCCI combustion, but different operating strategies should be implemented to ensure clean and efficient HCCI combustion according to the particular physical–chemical properties of different fuels. Lida et al. investigated the basic properties of n-butane HCCI combustion under different inlet temperatures, compression ratios, and engine speeds in a CFR engine [158]. Huang et al. evaluated the effect of spark discharge on n-butane HCCI operating limits using engine experiments and computational flame modeling. The results suggest that, with the elevated temperatures required to achieve HCCI combustion, the in-cylinder charge is capable of supporting a propagating flame over most of the HCCI operating regime [159]. Propane is available commercially for use in conventional internal combustion engines as an alternative fuel for gasoline. However, its application in developing HCCI combustion requires various approaches, such as high compression ratios and/or inlet charge heating, to achieve auto-ignition [160]. In addition to the aforementioned fuels, acetylene can also be used for HCCI combustion [161].

3.3. *Evolution of gasoline- and diesel-fueled HCCI combustion*

3.3.1. *Major pathways for gasoline HCCI combustion*

The modern HCCI combustion concept stems from ATAC, which was proposed by Onishi et al. [1] and Noguchi et al. [2]. Following this pioneering work, Najt and Foster applied this new combustion process to a four-stroke single-cylinder engine in 1983 [4]. After that, Thring further examined the effect of external EGR and air/fuel ratio on engine performance [162]. In this work, Thring introduced the terminology of ‘homogeneous-charge compression-ignition (HCCI)’ that has since been widely accepted by many other researchers to describe this type of combustion process both in gasoline and diesel engines. In 1992, Stockinger et al. [163] showed for the first time that a four-cylinder gasoline engine could be operated with auto-ignition within a very limited speed-load range using a higher compression ratio and intake charge preheating. The key obstacle to achieving HCCI/CAI combustion with commercial gasoline and other gasoline-like fuels with high octane number is that of raising the mixture temperature to the self-ignition or decomposition critical point before reaching TDC. In addition to intake charge preheating and increasing the compression ratio, residual gas trapping based on variable valve timing and/or lift has become a widely used control strategy. In this method, the thermal energy of residual gas is used to enhance the mixture temperature so as to control combustion phasing by the modulation of the residual gas fraction. It should be noted that not only the thermal energy but also a mass of CO_2, water vapor, CO, unburned HC, and radicals or intermediate species are contained in the residual gas. These species will partially change the reaction routes and reaction rates in the next operating cycle. These effects, including the heat capacity effect, dilution effect, and chemical effect, can also be used to control ignition and smooth the combustion rate at larger loads [164].

In most cases, the required conditions for gasoline HCCI combustion are created by internal exhaust gas recirculation (IEGR). Hot recirculated exhaust gas increases the charge temperature, causing cylinder temperatures to reach the auto-ignition temperature towards the end of the compression stroke. In general, IEGR can be grouped into five categories based on different forms of variable valve actuation and exhaust gas re-breathing. The first residual gas-trapping category is based on negative valve overlap (NVO) with earlier exhaust valve closing and later inlet valve opening. NVO is occasionally accompanied by a shorter valve event length and a smaller valve lift. The negative valve overlap method was realized by employing fully flexible variable valve actuation systems. By adjusting the valve open/close timing, the exhaust gas fraction and the real compression ratio can be controlled [165]. However, there is a drawback with the negative valve overlap approach. As the residual gases are recompressed and expanded, heat loss can take place from the hot residuals to the cylinder walls. As a result, a small pumping loop is produced. The second type of IEGR is referred to as late exhaust port recirculation (re-breathing) from the exhaust port [166]. This means that a second exhaust valve lift takes place at the end of the intake phase after fresh air is delivered to the cylinder. The burned gas then comes directly from the exhaust port. Again, the amount of internal EGR is controlled by the opening duration of the second exhaust valve lift. The third IEGR method uses a second opening of at least one exhaust valve in the early phase of the intake stroke. The burned gas is sucked directly from the exhaust port into the cylinder and mixed with fresh air from the intake side. The EGR rate is controlled primarily by the duration of the second exhaust valve lift [167]. The fourth IEGR method is known as intake port exhaust gas re-breathing. This method functions by blowing back the burned gas into at least one intake port by the early opening of at least one intake valve (as indicated by the second lift in the diagram). The opening timing and duration defines the amount of residual gas for the following cycle. In the suction stroke, burned gas plus fresh air is delivered to the cylinder [168]. Late exhaust port recirculation with dual exhaust valve opening, as well as the intake port recirculation strategy, offers a lower temperature in the cylinder. Intake port recirculation leads to a minimized stratification of fresh air and residual gas due to the homogenization of the residual gas starting with it being forced into the intake port. The last IEGR method is partially parallel exhaust port recirculation. It is employed with later exhaust valve closing and intake valve closing [169]. For the presented gasoline HCCI study, the extensive flexibility of the valve train is used to define the necessary variability in valve timing and the transition time between different operating modes of the valve train. However, the changing valve train activity is significantly influenced by the temperature history and spatial distribution of the residual gas from the previous combustion cycle, which further affects the auto-ignition behavior of the following cycle [170]. Yang et al. [171–173] proposed an optimized kinetic process (OKP) HCCI combustion concept that utilizes waste thermal energy contained in exhaust gases and coolant to preheat the intake air. By combining the intake/exhaust thermal management, VVT, and VCR technologies, a relatively high indicated thermal efficiency can be obtained across a wider operating range.

After many years of research, gasoline HCCI combustion still suffers from a narrow engine load operation range. To address this problem, methods such as intake charge boost [174,175], external EGR combined with internal EGR [176–178], spark-assisted ignition [179,180], and other methods have been used to expand the operating load. In general, HCCI combustion operated with no spark is necessary for stable operation with low NO*x* emissions, while spark-assisted has potential to improve the stability of HCCI combustion and expand the useful HCCI operating ranges. Additionally, mode switching between HCCI and traditional SI combustion has been implemented [181,182] so as to incorporate this advanced combustion mode into a practical commercial engine. For example, Shavor investigated the mode transition between SI/HCCI/SI on a test engine equipped with a variable valve actuation system [183]. Zhang et al. developed a four-valve variable actuation system that is capable of the independent control of the intake and exhaust valve lift and timings [184]. This was incorporated into a specially designed cylinder head for a single-cylinder research engine and a 4VVAS-HCCI gasoline engine test bench. The experimental research was carried out to study dynamic control strategies for transitions between HCCI and SI modes of the HCCI operating boundaries. It was found that switching from HCCI to SI operation is less problematic than is switching from SI to HCCI, and it was also demonstrated that the spark timing and exhaust valve closing timing have the largest effects and can be optimized for mode switching [185].

3.3.2. *Main approaches for diesel-fueled HCCI combustion*

Traditional mixing-controlled diffusion combustion features high fuel efficiency but high NO*x* and PM emissions. Despite the impressive progress made in the last decade, the diesel engine is still plagued by the well-known NO*x* and particulate trade-off [186]. It is obvious that such limits will require new advanced technologies and/or new combustion processes. A potential method for the simultaneous reduction of both NO*x* and soot outputs is to reduce the heterogeneity and flame temperature via new combustion methods. From a conceptual point of view, diesel-fueled HCCI would allow for a drastic reduction of particulates and NO*x* emissions to near-zero levels by using two basic processes: first, a homogeneous mixture has to be formed, and second, this mixture must auto-ignite due to compression heat. However, these same characteristics also present the main challenges. Diesel fuel is characterized by high viscosity, a wide range of boiling points, and a high cetane number. That means the required mixing timescale for creating a homogenous mixture is very long but the chemical ignition timescale is very short [187]. Furthermore, fuel-wetting of diesel-fueled HCCI engines is also a problem under consideration.

The major obstacles to diesel-fueled HCCI combustion are homogenous mixture preparation, the control of the ignition timing and combustion rate, and load range expansion. Diesel-fueled HCCI combustion can be implemented with various methods such as high-pressure multiple injections, high density or high boosting, controllable EGR, variable compression ratio, flexible fuel-supplying strategies, variable valve actuation, and fuel-reforming technology. Diesel-fueled HCCI combustion can be grouped by the following types: 1) port fuel injection, 2) early direct injection based on the combination of fuel bumping, small-diameter nozzle, narrow spray angle, and multiple injection, 3) late direct injection assisted by a high level of EGR and high swirl ratio, and 4) compound HCCI combustion with PFI combined with early direct injection. It should be pointed out that with regard to typical nomenclature for diesel-fueled HCCI combustion, many researchers prefer the term Premixed-Charge Compression-Ignition (PCCI) because, from a theoretical point of view, it is not possible to create a genuinely uniform mixture in so short a time duration.

Considering that a longer time duration is required for mixture preparation, fuel injection in the intake port is the most straightforward method used to prepare a homogeneous mixture, and the highest extent of homogenization is achieved by port fuel injection accompanied with intake charge preheating. This method is similar to that of PFI gasoline HCCI combustion. Whereas the basic goal of preheating for diesel HCCI combustion is to promote fuel evaporation and improve the mixture homogeneity, the purpose of preheating for gasoline HCCI combustion is to enhance the compressed temperature at TDC [188]. Recently, Musu et al. have proposed an innovative concept named Homogeneous Charge Progressive Combustion (HCPC) to control HCCI combustion in diesel-fueled engines [189]. The concept consists of forming a pre-compressed homogeneous charge outside the cylinder and gradually admitting it into the cylinder during the combustion process. In this manner, combustion can be controlled by the transfer flow rate, and high-pressure-rise rates, typical of standard HCCI combustion, can be avoided [190,191]. Results show negligible soot emission up to equivalence ratios near 0.85, with indicated efficiency of approximately 46%.

Late direct injection HCCI combustion refers to the HCCI mode in which injection occurs at a retarded crank angle compared to that of conventional diesel combustion, for example just before or behind TDC. Due to the expansion movement of the piston, the gas temperature and density decrease and lead to a longer auto-ignition delay to improve mixture formation. In addition, if high EGR rates are used to further extend ignition delay for the formation of premixed charge, soot and NO*x* formation can be simultaneously reduced due to the combustion temperature reduction. The classical late injection of HCCI combustion is the MK combustion system developed by the Nissan Motor Corporation [192–194]. To broaden MK operating ranges, a combination of prolonged ignition delay, shortened injection duration, higher pressure, a common-rail system, lower compression ratio, and cooling EGR was employed in the new-generation MK combustion systems.

Much more promising diesel HCCI combustion is achieved by early direct injection. At the end of the 1990s, the New ACE Institute in Japan proposed the PREDIC (PREmixed lean Diesel Combustion) [195–197] and MULDIC (MULtiple stage Diesel Combustion) combustion concepts [198,199], Toyota Motor Corporation developed the UNIBUS (UNIform BUlky combustion System) system [200–202], Hino Motors Ltd. developed the HiMICS combustion concept (Homogeneous charge Intelligent Multiple Injection Combustion System) [203], and Mitsubishi proposed the PCI (Premixed Compression-Ignition) combustion concept [204]. The common characteristic of these combustion systems is that the homogenous fuel/air mixture is created through sprays interacting via injector arrangement and nozzle design.

In the last decade, with the development of common-rail fuel injection systems and multi-hole injectors, direct injection systems now have the ability to flexibly control the fuel/air homogeneity and distribution. By equipping engines with a high-pressure common-rail system, Su et al. proposed a compound HCCI combustion concept that incorporates controlled premixed combustion and lean diffusion combustion [205–207]. At the Chalmers University of Technology, Helmantel et al. organized fuel/air mixture distribution and controlled combustion by five short injections during the compression stroke, with the start of the first injection set at 90 °CA BTDC [208]. At Shanghai Jiao Tong University, Shi et al. injected diesel fuel directly into the cylinder at intake TDC and adjusted the valve overlap to obtain a higher internal exhaust gas recirculation (EGR) in the cylinder [209,210]. Jacobs et al. investigated partially premixed compression-ignition, which was achieved by the use of an early injection, narrow spray-angle common-rail system in combination with EGR [211]. Kook examined PCCI combustion with two-stage early in-cylinder injection. It is interesting to note that in this work, the first injection was used as the main injection, but the second-stage injection with a small fuel quantity was used as an ignition promoter and combustion-phasing controller [212]. Since 2000, IFP has been working to solve diesel HCCI combustion problems and has developed the NADI™ (Narrow-Angle Direct-Injection) concept, a dual-mode engine that utilizes a highly premixed combustion (HPC) at low and medium loads and conventional diesel combustion at high and full loads [213–215]. A common-rail fuel injection system has been selected due to its continuously increasing flexibility, particularly in terms of injection events. A narrow spray cone angle was selected (approximately 70°) to limit fuel wall impingement and to promote fuel/air mixture, while giving large flexibility in terms of injection timing (very early or late injection). In addition, Pöttker, at the University of Hanover, promoted mixture formation with new nozzle geometry in combination with a multi-pulse injection scheme of up to nine shots with a highly flexible piezo-common-rail injection system [216]. In order to improve the mixture preparation and to avoid fuel loss due to wall impingement and the resulting unburned fuel, Ra et al. proposed a Variable Geometry Sprays (VGS) concept [217]. By numerical simulation, it was found that VGS is effective in minimizing wall wetting and allows wall wetting to be decoupled from ignition timing control.

3.3.3. Fuel design for diesel- and gasoline-fueled HCCI combustion

Due to fixed physical–chemical properties, traditional gasoline and diesel fuels may not be favorable for HCCI combustion. For gasoline HCCI combustion, it is necessary to equip engines with a complex valve actuation system to trap or re-breath exhaust gas. This complex system not only increases the production cost but also makes the engine control strategy more complex. For diesel fuel, low volatility and excellent ignitability make it difficult to broaden the engine load range and optimize engine thermal efficiency. IFP evaluated the effects on HCCI combustion of fuels with different cetane numbers ranging from 40 to 63 and with different boiling points and volatilities. The results showed that a low-CN fuel leads to a long auto-ignition delay, which allows more time for fuel vaporization and consequently yields better homogenization of the fuel, air, and residual gas mixture. High fuel volatility also favors the homogenization process. Moreover, it has been shown that, in addition to these classic physical properties, fuel composition highly impacts combustion behavior and therefore also affects noise and smoke emissions [218].

Both diesel fuel and gasoline fuel, in fact, are mixtures of various ingredients. Diesel fuel exhibits significant low-temperature heat release and staged heat release, as does gasoline fuel, with multi-stage heat release including a discernible low-temperature heat release [219]. According to fuel design principles, HCCI combustion control requires modulation of fuel components and the physical–chemical properties of gasoline and diesel fuel. For example, reduction of the boiling point and cetane number of diesel fuel can be accomplished by adding or blending inhibitors with lower boiling points, and the enhancement of gasoline cetane number can be achieved through the addition of a cetane number improver or the blending of high cetane number fuels. Through these modifications, the fuel/air mixture homogeneity and low-temperature reaction may be altered to some extent, consequently altering the overall combustion process. Bunting et al. [220] assessed the effects of cetane number (CN) on HCCI performance and emissions. Commercial fuels and blends of diesel secondary reference fuels were evaluated, covering a CN range from 19 to 76. Sweeps of intake air temperature showed that low-CN fuels required higher intake temperatures than did high-CN fuels in order to achieve ignition. The high-CN fuels exhibited a strong low-temperature heat release event while no LTHR was detected for fuels with CN values lower than 34. Odaka et al. [221] investigated the effect of diesel/MTBE blends on HCCI combustion. Widely used as a blend material for gasoline, MTBE is an oxygen-containing compound with a high octane number. It is characterized by a low boiling point, low vapor pressure, superb resistance to phase separation by water, and the absence of aromatic and olefin compounds, and thus, it can be expected to reduce smoke emissions. Its low boiling point facilitates the formation of homogeneous mixtures, and its low cetane number inhibits early ignition of the mixture. With an increase in MTBE content, the ignition timing of a mixture is retarded and combustion is initiated nearer to TDC. Additionally, combustion can be regulated using a DI fuel in the full-load operation range. Mohammadi et al. blended ethanol into diesel fuel, and realized PCCI combustion using a two-stage injection in which part of the fuel was injected during the compression stroke and the rest near TDC [222]. Gasoline fuel was injected into the intake port while dimethyl ether (DME), selected as an ignition promoter, was injected directly into the cylinder during the intake stroke and used to control the ignition and combustion [223].

Indeed, due to the complementary nature of the physical–chemical properties of diesel and gasoline, dieseline-fueled HCCI combustion is very attractive [224]. Gasoline, with its high volatility and easy vaporization and mixture formation, is used to form the homogeneous charge. Diesel fuel, which exhibits good ignitability and rapid combustion in the HCCI environment, is used to control the auto-ignition and restrain knocking combustion. It is expected that these two different fuels, with opposite but complementary properties, can be used to reach a good compromise for HCCI combustion. Zhong et al. investigated dieseline-fueled HCCI combustion under the condition of intake heating at compression ratio (CR) 15.0 and negative valve overlap (NVO) at CR 10.4 [225]. The experimental results revealed that, with an increasing proportion of diesel fuel in the blend, the intake temperature required for knock-free HCCI operation was lowered, the lower end of the IMEP range possible with the NVO and the excess air ratio range were all extended, and HC and NO*x* emissions were greatly reduced throughout the engine load range. Moreover, improved combustion stability was obtained with gasoline/diesel-blended fuel as compared with gasoline-fueled HCCI. The HCCI combustion region was expanded dramatically without a substantive increase in NO*x* emissions under given inlet and exhaust valve timing due to the improvement of charge ignitability resulting from the addition of diesel fuel [226]. Weall et al. demonstrated that a combination of fuel properties exhibiting higher volatility and increased ignition delay would enable extension of the low-emission operating regime [227]. An increased proportion of gasoline fuel also reduced smoke emissions at higher operating loads through an increase in charge premixing resulting from an increase in ignition delay and higher fuel volatility. Turner et al. compared the HCCI combustion of neat gasoline and 10% and 20% gasoline/diesel blends [228]. It was shown that the lean limit of excess air ratio can reach almost 2.0 when the engine is operated with moderate compression ratios. The combustion of the blended fuel offers promise for achieving the desired ignition quality, which reduces the dependence of HCCI on EGR trapping or intake heating for a wide range of compression ratio.

4. Real-time fuel design for HCCI combustion

4.1. Dual-fuel HCCI combustion

Previous section has shown that HCCI combustion can be expanded to a wider load-speed operating range by the use of fuel additives or fuel blending when compared to single ingredient fuels, which are not suitable for large- to full-load-speed HCCI operating ranges. From an ignition control and load expansion point of view, a high cetane number fuel is suitable for low load and cold start while a high octane number fuel with anti-knock capability is preferable for large to full loads. Furthermore, an optimum octane number exists that yields the highest indicated thermal efficiency for a certain operating case [229]. To achieve this target, an effective method for the optimization of the overall operating process is the use of a dual-fuel HCCI combustion system. In general, the first step in a dual-fuel HCCI combustion system is to select a group of test fuels with opposite chemical properties. A fuel with a low boiling point and a high cetane number (such as DME or n-heptane) is selected as an ignition improver, while a high octane number fuel (such as gasoline, LPG, methanol, ethanol, or CNG) is selected as an ignition suppressor. By selecting two fuels with opposite properties, HCCI combustion can be flexibly controlled using open- or closed-loop control strategies.

Yeom et al. investigated gasoline-DME and LPG-DME dual-fuel HCCI combustion [230,231]. Liquefied petroleum gas (LPG) and gasoline were injected into the intake port using port fuel injection equipment. Dimethyl ether (DME) was used as an ignition promoter and was injected directly into the cylinder during the intake stroke. The authors found that LPG is more suitable for the high-load operation of HCCI than is gasoline because of its high latent heat of vaporization and octane number. Additionally, the knock intensity of the LPG-DME combination was lower than that of gasoline-DME. Yao et al. investigated DME-methanol dual-fuel HCCI combustion in a single-cylinder engine. The ignition timing and combustion duration could be regulated within a suitable range, with high indicated thermal efficiency and low emissions, by adjusting the DME percentage and EGR rate [232]. The key aspects of this dual-fuel HCCI combustion are the EGR control strategy and DME percentage applied simultaneously at each operating point [233]. Furthermore, they also conducted an experimental HCCI combustion study of port fuel injection DME with the direct in-cylinder injection of methanol [233]. The active radicals and heat release during the LTR and HTR of the premixed DME triggered the ignition and combustion of methanol. The combustion rate may be altered by varying the in-cylinder injection timing. Konno et al. measured and analyzed the intermediate species produced in DME/methane HCCI combustion [234]. Sato et al. also researched methane/DME/air pre-mixture HCCI combustion and examined the associated oxidation reaction routes [235]. Jang et al. investigated DME/LPG HCCI combustion with the port fuel injection of LPG and the in-cylinder direct injection of DME during the intake stroke [236]. They then compared the combustion characteristics of different fuel strategies: port fuel injection LPG with the in-cylinder injection of DME and port fuel injection DME with the in-cylinder injection of LPG. The results showed that DME direct injection with LPG port injection resulted in later combustion as compared to LPG direct injection with DME port injection. This made an increase in DME and LPG fuel quantity possible, which resulted in a wider operating region [237].

DME-CNG dual-fuel HCCI combustion is also characterized by a distinctive two-stage heat release process. As the CNG flow rate increases, the magnitudes of the peak cylinder pressure and peak heat release rate in the second stage also increase. As the DME flow rate increases, the peak cylinder pressure, heat release rate, and NO*x* emissions increase while THC and CO emissions decrease. Use of a dual-fuel is an effective technique for controlling HCCI combustion and extending the HCCI operating range by adjusting fuel proportion [238]. Olsson et al. demonstrated the possibility of achieving high loads, up to 16 bar BMEP, and ultra-low NO*x* emissions of ethanol/n-heptane dual-fuel HCCI combustion on a six-cylinder turbocharged truck engine [239]. The maximum efficiency achieved in this study was 41.2%, which is slightly lower than that of the original diesel engine. Furthermore, this combustion system suffered from two problems: the first was lower combustion efficiency at lower loads due to the lack of inlet air preheating, and the second was higher pumping losses at high loads due to the low exhaust temperature. A variable geometry turbocharger was employed to overcome these problems, and an overall net indicated efficiency at a high load between 45% and 50% was obtained using turbocharged operation [240].

Dual-fuel HCCI combustion may be quite troublesome (complex) in actual practice, as it is necessary to equip engines with two fuel supply systems. Therefore, fuel reforming was proposed for control of HCCI combustion by generating multiple fuel components with the use of one fuel supply system. Fuel reforming involves the catalytic reaction of engine exhaust gas (a source of oxygen and steam at high temperature) with hydrocarbon fuel to produce hydrogen, CO, and other small molecules that can then be recycled to the engine as reformed exhaust gas recirculation (REGR). The reactions include complete and partial oxidation reactions and steam reforming reactions as well as the water/gas shift reaction. These reactions may be accompanied by others, such as the dry reforming reaction (endothermic reaction of fuel and carbon dioxide that occurs at high temperatures and produces hydrogen) and coke-forming reactions. Although CO and HC are difficult to auto-ignite, CO is an intermediary product of the combustion process and may be completely oxidized to CO_2 at 1500 K, and H_2 has the ability to improve local combustion in efforts to alter the overall ignition and combustion process of primary fuels. Given the large differences in fuel components and fuel chemical properties between the reformer gas and base fuel, the resulting ignition and combustion control mechanism is similar to that of the dual-fuel system. For this reason, this paper recognizes reformer gas HCCI combustion as one type of dual-fuel HCCI combustion. It is worth noting that the effects of the RG on HCCI combustion rely on many factors, such as the CO/HC ratios of the RG, the replacement fraction, base fuel auto-ignition characteristics, in-cylinder environment, mixture thermodynamic properties, and mixture chemistry [241].

Hosseine et al. investigated the effects of reformer gas fuel replacement on HCCI combustion in a CFR engine with iso-octane and PRF80 [242]. In the experiments, a simulated gas (75% H_2, 25% CO) was used to alter the HCCI combustion characteristics. The results indicated that combustion was retarded by increasing the RG fraction in the base fuel. This reduced the maximum cylinder pressure and maximum cylinder pressure-rise rate, leading to a smoother combustion. However, the thermal efficiency was reduced slightly due to the increased CO and HC emissions. For a high cetane number fuel, such as n-heptane or PRF20, replacing some of the base fuel with reformer gas generally expands the engine operating range on the rich side and retards combustion timing [243]. Yap et al. [244] and Peucheret et al. [245] introduced exhaust reforming gas into the cylinder to control CNG HCCI combustion. It was found that one important advantage of REGR addition is that much lower loads can be achieved for a given intake temperature. Moreover, when REGR was introduced, NO*x* emissions exhibited a decrease, but CO and HC emissions were increased. In general, use of reforming gas has the capability to adjust HCCI ignition timing and the heat release rate by varying the fraction of reformer gas. This approach offers a potential combustion control mechanism at the expense of CO and HC emissions.

Hosseini et al. further examined the variation of the H_2/CO ratio and RG composition in n-heptane, iso-octane, and CNG-based HCCI combustion [246]. For all three fuels, RG blending was able to provide combustion-timing control despite the wide range of reformer gas composition. It was found that for CNG-fueled HCCI combustion, the use of RG advanced the combustion timing significantly, but its components showed no obvious effect on the ignition phasing. RG can be used to expand the natural gas HCCI combustion operating window on the lean side when the H_2 content of the RG is high. For iso-octane-fueled HCCI combustion, the effects of RG are small and depend greatly on the temperature. In the case of higher compressed temperatures, RG blending will raise the compression temperature and lead to earlier combustion timing. In the case of moderate initial conditions, however, RG blending retards the combustion timing. For n-heptane HCCI combustion, H_2 and CO have a similar effect on the suppression of low-temperature oxidation kinetics. The effect of the reformed gas component on HCCI combustion was a significant difference between real and simulated reformed gas. Toshio et al. proposed an HCCI combustion engine system fueled with dimethyl ether, which has a high cetane number, and methanol-reformed gas (MRG), which has a superior anti-knock property. Both DME and MRG are produced from methanol by onboard reformers utilizing the exhaust heat from the engine. As the reactions producing DME and MRG are endothermic, a part of the exhaust heat energy can be recovered during the fuel-reforming process so as to improve energy utilization [247].

4.2. Real-time fuel design for HCCI combustion with PRFs

In general, to characterize an acceptable HCCI operating range, certain criteria for acceptable operating points have been used as follows: (1) ignition reliability under cold start and lower loads at low engine speeds, (2) combustion efficiency and operating stability under lower loads at middle-to-high engine speeds, (3) NO*x* criteria at large loads, and (4) noise level and volumetric efficiency at higher engine speeds. During HCCI engine run, cycle-to-cycle variations and cylinder-to-cylinder variations are always observed at leaner fuel/air mixtures or lower engine loads regardless of whether a high cetane number fuel is used [248]. Under larger loads or a richer fuel/air mixture, misfire and incomplete combustion induced by the poor ignitability are also occasionally observed [249,250]. To obtain higher power density, lower NO*x* emissions, and maximum thermal efficiency, it would be better to alter the fuel properties including fuel ignitability and anti-knock index from cycle-to-cycle, according to operating conditions and in-cylinder combustion characteristics [251], or in other words, to implement fuel design in real-time.

In the traditional fuel design method, gasoline or diesel fuel properties are altered by fuel blending or the addition of a fuel additive before being supplied to the fuel injection system [252]. In essence, fixed proportion fuel blending is similar to that of the original base fuel and is often unable to match the chemical reaction kinetics for controlled HCCI combustion; it is also difficult to achieve mode transitions and heat release modulation over wide operating conditions. As a result, the problems of uncontrollable combustion, a narrow speed-load range, and the trade-off between emissions are not solved. Moreover, conventional dual-fuel HCCI combustion pays little attention to the cold start, cycle transition, and cycle-to-cycle and cylinder-to-cylinder variations. The control strategy is open-loop. Real-time fuel design aims to change the fuel physical–chemical properties from cycle-to-cycle and cylinder-to-cylinder by altering the fuel blending proportion so as to modulate the required mixing and ignition timescales in real time [253]. When combined with in-cylinder closed-loop feedback control based on detailed combustion information, optimized combustion phasing, combustion mode, heat release pattern, emissions, and thermal efficiency can be achieved.

For an n-heptane/iso-octane dual-fuel HCCI combustion system, by combining the ignitability characteristics of n-heptane and the anti-knock capability of iso-octane, the n-heptane/iso-octane proportions can be modulated in real time according to the operating conditions and combustion characteristics of the previous cycle. For example, this can be accomplished by supplying only n-heptane at cold start but adding a moderate iso-octane proportion as the load increases while maintaining CA50 near TDC and ensuring ignition stability. From medium to large loads, a large proportion of iso-octane can be added to improve the overall anti-knock capability and enlarge the operating load range. Based on this strategy, the maximum in-cylinder pressure and center point of the heat release are allowed to occur near TDC through the control of the low-temperature reaction by altering fuel properties and quantities, as shown in Fig. 12. The results include an expanded engine load range, smooth heat release, reduced pressure-rise rate, improved thermal efficiency, and reduced engine emissions. Fig. 13 shows the n-heptane/iso-octane real-time fuel design experimental system.

In the case of HCCI combustion with neat n-heptane, the maximum IMEP is less than 0.25 MPa but is expanded up to 0.47 MPa using optimized n-heptane/iso-octane proportions in real time [254]. Fig. 14 shows the optimized routes of the n-heptane/iso-octane proportion and thermal efficiency. Regarding emissions, HC emissions of the optimized running routes are maintained at a level of 150–350 ppm for all engine loads, and CO emissions are lower than those associated with fixed blended fuel or neat fuel. Additionally, NO*x* emissions are almost zero at all optimized running ranges [255].

4.3. Real-time fuel design for HCCI combustion with DME and LPG

The composition of LPG affects DME-LPG dual-fuel HCCI combustion due to differences in the physical–chemical properties of propane and butane, such as octane number, auto-ignition temperature, and the heat of vaporization. In general, the power output may be moderately increased by a larger propane concentration due to increased expansion work and improved anti-knock properties. However, with a higher propane proportion, combustion efficiency is decreased because of suppression of the low-temperature reaction of DME, which determines the heat release amount in the high-temperature reaction [256]. Jiang et al. compared two different DME-LPG dual-fuel HCCI combustion modes, port fuel injection of LPG with in-cylinder direct injection of DME and port fuel injection of DME with in-cylinder direct injection of LPG [236]. The results showed that DME direct injection with LPG port injection was the better of the two methods for increasing IMEP and reducing emissions; this was due to the observation that auto-ignition timing was controllable with the modulation of the direct injection timing. In the case of port injection with a high cetane number fuel, performance was limited due to the appearance of an excessively early combustion phase as the amount of fuel injection was increased. Therefore, a possible method for optimizing DME-LPG dual-fuel HCCI combustion may be real-time fuel design, which can be used to change the fuel

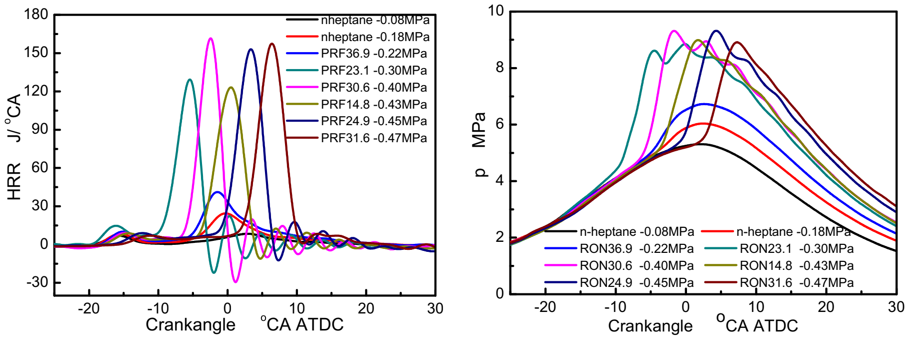

Fig. 12. Main operating points of real-time optimized n-heptane/iso-octane HCCI combustion.

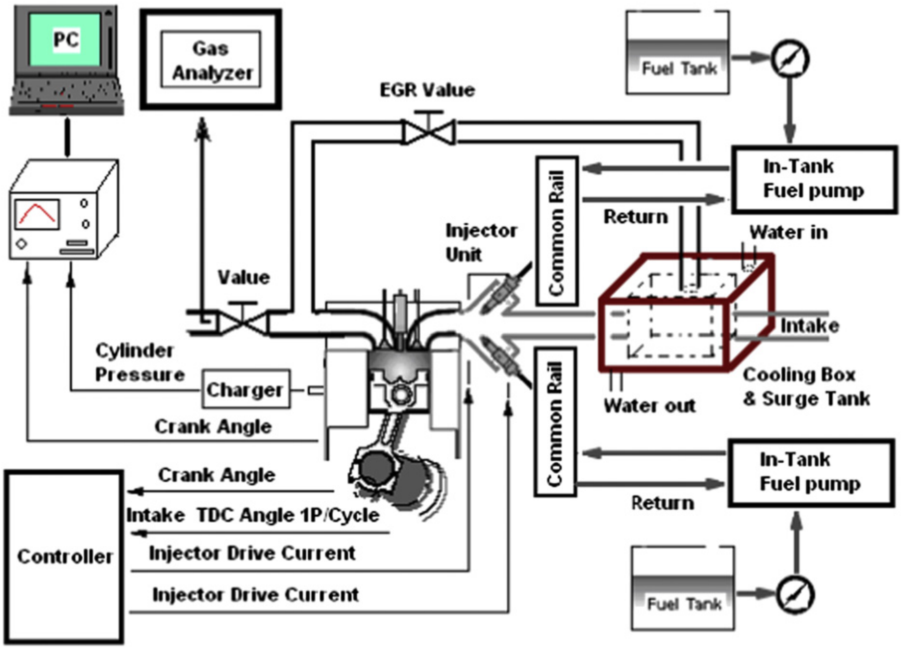

Fig. 13. Experimental setup for n-heptane/iso-octane real-time fuel design.

proportion according to combustion information and operating conditions [257].

By integrating the excellent ignitability of DME and the anti-knock capacity of LPG, detailed combustion characterized parameters—including start point and peak point of cool flame, NTC duration, combustion phasing and peak value of hot flame, and maximum in-cylinder pressure and its crank angle—can be flexibly modulated through the control of the DME/LPG proportion. A smooth and concentrated heat release is observed as a result, as seen in Fig. 15. Fig. 16 compares the thermal efficiency and maximum BMEP of DME HCCI combustion using different strategies. This figure shows that, by optimizing the DME/LPG proportion, the maximum BMEP is enlarged from 0.16 MPa in neat DME HCCI to 0.47 MPa, and the thermal efficiency is optimized for overall operating ranges [258].

5. Evolution of low-temperature combustion

5.1. Principles and basic characteristics of low-temperature combustion

Although it has been employed with high-pressure common-rail electronic fuel injection systems in combination with ultra-multi-hole and multi-pulse injection schemes, diesel-fueled HCCI combustion is still faced with the obstacles of narrow operating ranges, short ignition delay, difficult non-homogenous mixture formation, and several other problems. In essence, the key aspects of HCCI combustion depend more on the mixture homogeneity, whereas the thermal efficiency and emission levels of practical engines are decided by detailed information regarding the overall combustion event, rather than only by mixture homogeneity. Many studies have revealed that in-cylinder combustion temperature plays a crucial part in the formation and evolution of emissions as well as thermal efficiency. Near the year 2000, several researchers introduced a new method used to depress NO*x* and smoke formation by controlling the combustion temperature [259]. It is accepted that one way to avoid both soot and NO*x* emissions is to keep the temperature during combustion below about 1650 K. In this way, both the NO and soot formation zones are completely avoided regardless of the equivalence ratio. Since then, a new combustion concept known as low-temperature combustion (LTC), which is formed on a similar basis to HCCI combustion, was proposed by Sandia National Laboratories [260], the University of Illinois at Urbana-Champaign [261], and other research institutes. LTC utilizes high levels of dilution (EGR $>$ 60% or $<$10% O_2 in the intake charge) combined with flexible fuel injection strategies and

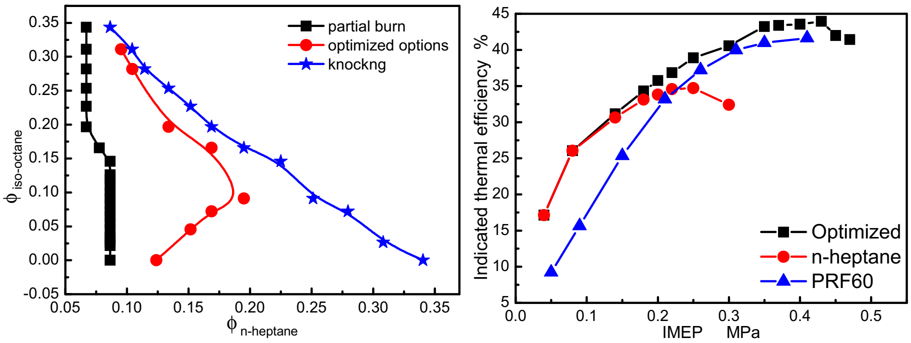

Fig. 14. Optimized run pathway and emissions for n-heptane/iso-octane HCCI combustion.

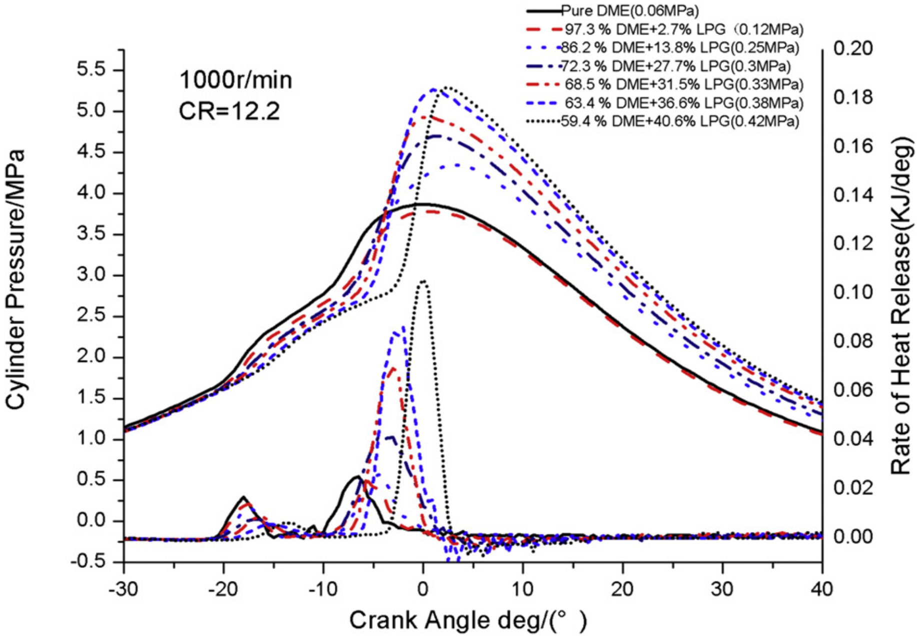

Fig. 15. LTR and HTR of DME-LPG dual-fuel HCCI combustion using real-time fuel design.

strongly turbulent in-cylinder conditions to reduce overall combustion temperatures to those below the critical point of NO*x* and smoke formation. In 2005, a university consortium, consisting of the University of Michigan, the Massachusetts Institute of Technology, Stanford University, and the University of California-Berkeley, was founded and devoted to LTC research [262]. In recent years, the University of Wisconsin–Madison, Brunel University, Windsor University, Chalmers University of Technology, and others have conducted fundamental studies on this combustion mechanism.

LTC, also known as dilution-controlled combustion, is different from high-temperature combustion (HTC), which is dominated by fuel/air mixing, and also from HCCI combustion, which is dominated by fuel/air chemical kinetics. Compared to HTC, LTC forms a more uniform mixture before spontaneous ignition. However, compared to HCCI combustion, it employs high levels of EGR and moderate inhomogeneity of whole mixtures. Its most prominent characteristic is that turbulence and mixing play an important role in combustion and emissions as well as in fuel/air chemical kinetics. The combination of these two combustion modes makes it a unique method that can be used to retain high thermal efficiency and smooth heat release. LTC also differs from SCCI (or PCCI) combustion in that it utilizes high levels of dilution (EGR $>$ 60% or $<$10% O_2 in the intake charge) combined with fuel injection strategies in addition to strong in-cylinder turbulence and mixing to control overall combustion temperatures. The major purpose of dilution is to lengthen the ignition timescale [263], and this increased ignition delay provides time for fuel evaporation and reduces inhomogeneities in the reactant mixture. Fuel strategies and turbulence are employed simultaneously to shorten the mixture preparation timescale, thus reducing NO*x* formation from local temperature spikes and soot formation from locally rich mixtures. Furthermore, low oxygen concentration reduces the adiabatic flame temperature substantially [264] so as to make the in-cylinder combustion temperature lower than the critical point of smoke and NO*x* formation [265]. Fig. 17 displays the difference between the diesel combustion modes.

5.2. *Key points of low-temperature combustion*

To achieve LTC in compression-ignition engines, the most important requirement is to inject all fuel into the cylinder and promote homogenous mixture formation prior to spontaneous ignition. This requires a longer ignition delay, which is achieved by a high level of EGR or a lower oxygen content. Furthermore, strong in-cylinder turbulence is preferred to create a uniform mixture. Third, LTC requires a flexible fuel strategy. Current global investigations are focused on the required fuel spray strategy, turbulence

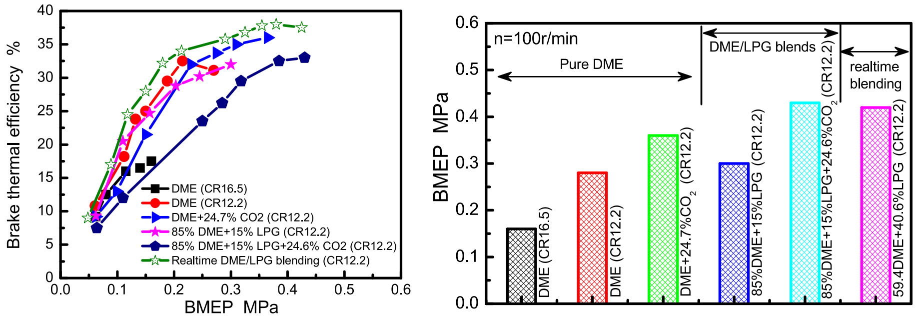

Fig. 16. Brake thermal efficiency and expanded engine load for DME/LPG dual-fuel HCCI combustion under different strategies.

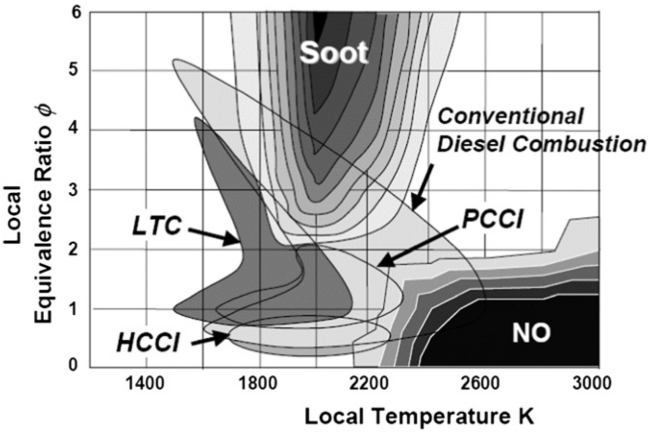

Fig. 17. Comparison of diesel fuel combustion modes in a ϕ–T diagram [266].

and mixing intensity and their effects, EGR or low oxygen operating mechanism, optimization of the engine parameters, and so on.

5.2.1. *Fuel strategy and its effects*

Due to the higher boiling ranges and lower volatility of diesel fuel in addition to its good ignitability, it is necessary to precisely control the fuel injection strategies. Martin et al. [267] employed an ultra-multi-hole injector with small-diameter orifices to promote mixture homogeneity. The dual-row, narrow-included angle nozzle provided the spray targeting necessary to contain the direct-injected diesel fuel within the piston bowl for injection timing as early as 70 °C BTDC. Fang et al. [268] found that increasing injection pressure can greatly reduce soot emissions. However, lowering injection pressure is helpful, to some extent, in reducing combustion temperature, which improves NO*x* reduction. For this reason, lower injection pressure is preferred at higher loads. In these cases, liquid fuel is injected into a low-temperature premixed flame, which is different from conventional diesel combustion with liquid fuel injected into a hot premixed flame. The author further investigated the effects of injection angles on low-temperature combustion within an optically accessible HSDI diesel engine by employing pre-TDC in-cylinder injection or post-TDC injection strategies [269,270]. The results show significant influences of injection angles on the air–fuel mixing process and combustion characteristics. With narrow-angle wall-guided sprays, the injection timing can be significantly retarded to implement low sooting combustion compared with conventional spray combustion [271,272]. The late post-TDC injection strategy and pre-TDC early injection strategy with very early injection timings show better performance in reduction of both NO*x* and soot. However, as far as the fuel consumption is concerned, the pre-TDC very early injection strategy has poor fuel efficiency with significantly higher fuel consumption than the post-TDC late-injection strategy cases. The late post-TDC injection strategy shows the best performance in terms of soot emissions, NO*x* emissions, and fuel efficiency [269]. Zheng et al. suggested that single-shot injection with prolonged EGR is suitable for low loads, while two to five shots of late early injection is recommended for medium loads, and six to eight shots and EGR should be used for high loads [273]. Bobba et al. [274] found that a combination of high EGR and post injections has potential to reduce soot emissions effectively while maintaining low NO*x* emissions. In addition, due to the substantial effect of the high EGR on heat release, complex combustion modes that characterize clean and efficient combustion techniques should be modulated by altering the injection pulse and injection timing for different EGR level so as to move CA50 near the top dead center [275].

5.2.2. *Mixture turbulence and mixing*

Both the ignition and mixing timescales of the fuel/air mixture dominate LTC emission and combustion characteristics. For this combustion mode, intensive in-cylinder turbulence has an important positive effect on shortening the fuel/air mixing timescale. Su proposed a timescale-controlled combustion concept that employs large-scale turbulence induced by combustion chamber design combined with multi-pulse fuel injection during the early period to control the mixing and chemistry timescales and overall combustion path [276]. Choi et al. evaluated the impact of swirl ratio, varied from 1.44 to 7.12, on late-injection, low-temperature combustion. The results revealed that variation in flow swirl impacts the latter half of the combustion process and affects the initial combustion only slightly. An optimum Ricardo swirl ratio was found to exist for the best moderate-load efficiency and soot oxidation [277]. Noehre et al. found that the combination of low compression ratio, high EGR rate, higher intake boosting, and engine operation close to stoichiometric conditions enables simultaneous NO*x* and soot reduction, up to 15 bar IMEP gross. The reason for this seems to be a combination of improved fuel vaporization and air entrainment due to the higher in-cylinder pressure at the moment of injection. In summary, the low soot emissions in these methods seem to be a result of good premixing, long ignition delay, and low local combustion temperature [278]. Pickett investigated low flame temperature limits for mixing-controlled diesel combustion in a constant-volume combustion chamber. By varying ambient oxygen concentration or by using fuel-lean mixing-controlled combustion, combustion efficiency remained high for adiabadic flame temperatures as low as 1500–1600 K [279].

5.2.3. *Effects of EGR on LTC*

Zheng et al. found that a minimum mixing duration of 1.5 ms was sufficient to produce low NO*x* and low soot for multiple-injection strategies, but a longer ignition delay was required for a single-shot injection and EGR-enabled LTC [280]. The most efficient method used to prolong ignition duration is to employ a heavy EGR level. That is, EGR is the key aspect for LTC. Colban et al. assessed the influence of the EGR chemical composition on emissions behavior [281]. The simulated results revealed the importance of including H_2O, CO, and UHC. H_2O was observed to reduce ignition delay, UHC, and CO emissions while increasing soot emissions. CO was noted to increase ignition delay, UHC, and CO emissions while having little effect on soot emissions. For biodiesel, an increased CN results in a shortened ignition delay period, thereby allowing less time for air/fuel mixing prior to the premixed burning phase. Consequently, a weaker mixture is generated and burned during the premixed phase. Thus, ultra-low engine-out levels of NO*x* and soot were achieved by supplementing with 55%–65% EGR [282]. Kook et al. investigated the effect of charge dilution on LTC via simulated EGR varied from 0 to 65% [283]. Ogawa achieved ultra-low NO*x* and smokeless operation at higher loads, up to half of the rated torque, by applying large rates of cold exhaust gas recirculation (EGR) [284]. They found that NO*x* decreases to below 6 ppm (0.05 g/kW-h) and soot significantly increases when oxygen concentration is first decreased to 16% with cold EGR (40% EGR). However, after peaking at 12–14% oxygen (50%–55% EGR), soot formation then decreases sharply to essentially zero at 9–10% oxygen (60% EGR) while maintaining ultra-low NO*x*, regardless of fuel injection quantity and injection pressure. A further increase in EGR beyond a critical point resulted in increased cycle-to-cycle variation [285]. In particular, at higher loads, with the oxygen concentration below 9–10%, the air–fuel ratio must be over-rich to exceed half of the rated torque, in which case thermal efficiency, CO, and THC deteriorate significantly. Under these conditions, the promptness and accuracy of combustion control as well as tightened control on the intake oxygen concentration can enhance the robustness and efficiency [286].

5.2.4. *CO and HC formation mechanism*

A large number of studies have discovered that low-temperature combustion, which is assisted by high proportions of EGR, is capable of reducing NO*x* emission on a large scale and is almost smoke-free, although it is always accompanied by a high level of CO and HC emissions. The higher UHC and CO emissions can be attributed to the following reasons: lean-burn or combustion deterioration due to the heavy EGR, misfires at local lean or rich equivalence ratios, flame extinguishment in the piston-cylinder gap, and fuel-wetting on the surface of the combustion chamber. Furthermore, stratification of mixture temperature due to evaporation cooling and wall heat transfer significantly affects UHC/CO emissions in LTC engine operation [287]. Colban revealed that most of the UHC mass exits the cylinder during the latter part of the exhaust process, indicating that UHCs originating from the cylinder wall and piston-top quench layers are likely of greater importance than UHCs emitted from quench layers along the head [288]. Kim identified CO and HC sources using two-dimensional planar laser-induced fluorescence (PLIF) and evaluated the effects of oxygen concentration and injection timing on the spatial distribution of CO and HC emissions [289]. The major contributions to UHC from the clearance volume stem from regions near the cylinder centerline and near the cylinder wall, where UHC likely emanates from the top ring-land crevice. However, broadly distributed CO within the squish volume dominates CO observed near the cylinder centerline. Colban et al. further compared the HC/CO emissions and thermal efficiency of dilution-controlled LTC and late-injection LTC [290]. For both LTC strategies, increased intake pressure reduces emissions of unburned hydrocarbons (UHC) and CO, with corresponding improvements in combustion efficiency and indicated specific fuel consumption. Late-injection LTC offers improvements in engine noise and soot over dilution-controlled LTC. Conversely, dilution-controlled LTC yields lower emissions of UHC and CO as well as better combustion efficiency and thermal efficiency when compared to late-injection LTC. By examining in-cylinder UHC and CO images, Ekoto et al. discovered three main UHC source regions: centerline, squish volume, and bowl/central clearance volume [291]. Where squish volume UHC and CO principally result from the partial oxidation of the lean mixture and are the dominant sources of CO and significant sources of UHC. The nozzle region is a significant source of UHC but not of CO. CO is more abundant in the region close to the piston top, and UHC formed at the ring-land crevice is not an important source at the light load considered [292].

5.2.5. *Thermal efficiency of LTC*

Clean LTC combustion in terms of low regulated emissions can be established through the use of an exhaust oxidation catalyst to remove the engine-out total unburned hydrocarbon (THC) and carbon monoxide (CO) emissions [293], whereas the fuel efficiency of low-temperature combustion cycles was commonly compromised by high levels of hydrocarbon and carbon monoxide emissions. Thus, achieving the maximum thermal efficiency considering HC/CO emissions, heat release patterns, combustion phasing of CA50, load expansion, and other parameters has become an important issue. To identify the pathways for improved fuel efficiency of diesel LTC cycles, Kumar et al. analyzed the impact on the thermal efficiency of heat release phasing, duration, shaping, and splitting using zero-dimensional engine cycle simulations [294]. The results indicated that combustion phasing dominates the maximum attainable fuel efficiency of the engine. However, the use of heavy EGR resulted in a significant drop in combustion efficiency. An appropriate selection of injection strategy commensurate with boost and EGR levels offers a manner in which to avoid fuel condensation and wall impingement of fuel injected early during the compression stroke, and this will have a positive effect on thermal efficiency. Asad et al. attempted to optimize the thermal efficiency by modulating the heat release mode with flexible fuel strategies [295]. Empirical studies have suggested that a single shot with heavy EGR at low loads and multiple early-injections for medium loads are preferred. Zheng et al. proposed an energy-efficient biodiesel LTC mode solution using adaptive control of SOI and EGR strategies combined with intake charge boosting and high-pressure injection [296,297]. Su et al. found that high charge density can play a role in the increase of heat capacity along with exhaust gas recirculation (EGR) [298]. Therefore, low-temperature combustion can be realized with less EGR (approximately 18–19% oxygen concentration) in order to achieve very low NO*x* and soot emissions, which are extremely important at high and full loads. In addition, high charge density affects the fuel air mixing rate so as to promote the burning rate, particularly in the later phase of engine combustion, which leads to higher efficiency. Thus, the high density-low temperature combustion (HD-LTC) demonstrates potential for high thermal efficiency and very low engine-out emissions, as shown in Fig. 18. While, it should be noted that the PM emissions increased moderately at an oxygen content of 18%, this may be attributed to the impact of boost and injection pressure variation on the amount of liquid fuel remaining in the nozzle [299]. Henein et al. summarized the pathway used to improve the thermal efficiency in a series of steps [300]. The first of these steps is to advance the peak point of the premixed heat release to near TDC so as to improve the economy while increasing the NO*x* emissions. Then, increasing EGR to reduce NO*x* will cause an incremental increase in soot emissions. The third step is to increase the injection pressure and/or swirl ratio to decrease the soot. The fourth step is to optimize LPPC (location of the peak rate of heat release due to the premixed combustion fraction), injection pressure, and swirl ratio. In general, this approach requires a burn angle optimum for power output, which approximately corresponds to

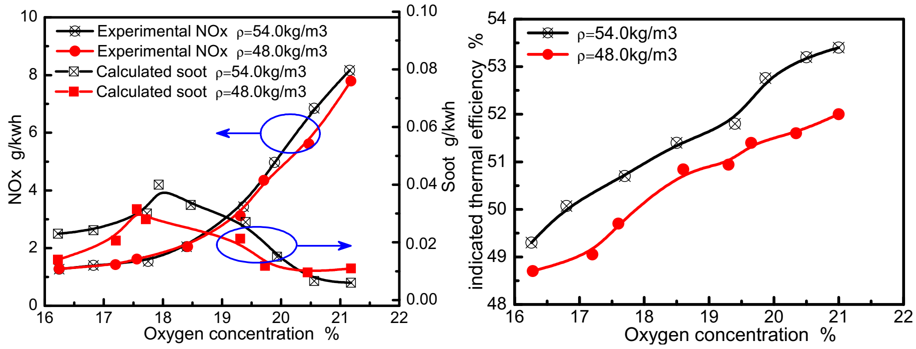

Fig. 18. Thermal efficiency and emissions of high-density-low-temperature combustion [298].

a CA50 between 3 and 10 °CA ATDC, and an ignition delay of 1.2–1.5 ms for sufficient mixing [301].

5.3. *Effect of fuel properties on low-temperature combustion*

For high cetane number but lower-volatility diesel-type fuels, high-pressure multiple-split injection and high level dilution are employed to balance the local and overall mixing times (τ_1) as well as the chemistry times (τ_2). Longer mixing times generally yield more homogeneous mixtures and improve PM emissions. However, to extend the mixing time, the chemistry timescales must also be extended so that ignition does not occur prior to the desired level of premixing. Furthermore, it is apparent that if air–fuel mixing rates can be increased, the necessary mixing times and ignition delay requirements can be reduced, thus gaining more control over combustion phasing. In other words, fuel chemistry plays a significant role in the ignition delay duration as well as determining overall combustion characteristics and emissions. Cheng et al. designed five blends of conventional diesel fuel and a high volatility (HV) fuel mixture of n-heptane and toluene, all of which had approximately the same ignition quality [302]. They found that increasing the HV fuel content was an effective means of reducing or eliminating liquid-fuel films and pool fires. Small increases in the HV content produced large changes under conditions where pool-fire activity was significant. For the LTC conditions studied, an HV content of 78% eliminated pool fires and reduced smoke emissions to near-zero levels. As the cetane number of the test fuel dominated the ignition delay duration, Ickes et al. demonstrated the manner in which variations in fuel cetane number affect the detailed combustion behavior of premixed LTC [303]. Fuel cetane number was found to affect ignition delay and combustion phasing, and small deviations in combustion phasing can shift the combustion to less optimal modes. Warey et al. examined the influence of cetane number (CN) and other fuel properties on low-temperature combustion [304]. Butts et al. [305] investigated the effects of cetane number, volatility and total aromatic content of diesel fuels on LTC operation. The author found that Increasing CN reduces CO, HC, and ISFC while NO*x* and particulate emissions remain very low, increasing volatility significantly reduces HC emissions and particulates over the base fuel, increasing aromatic content does not cause a significant change in particulate matter at these conditions compared to the base fuel. Mueller et al. [306] researched the biodiesel-diesel blends and primary reference fuels with different cetane number on NO*x* emissions. In general, lower cetane number fuels demonstrated reduced NO*x* and smoke emissions in the low-temperature combustion regime due to their longer ignition delay but had higher HC and CO emissions. Additionally, it could be possible to extend the high load limits with further optimization of the injection strategy and engine operating parameters.

One major objective of the mixing-controlled LTC strategy is to reduce the local combustion temperatures and equivalence ratio at the liftoff cross-section. Then, oxygenated fuels such as biodiesel have an advantage in efforts to achieve smoke-free LTC combustion supplemented with a lower EGR rate due to their self-oxygen content [296,307–310]. This represents a substantial improvement on the combustion stability and cycle-to-cycle and cylinder-to-cylinder variations. Another method used to improve mixing-controlled LTC is the promotion of mixture uniformity by blending gasoline and diesel fuel in different proportions. By using dieseline combined with a moderate EGR level, the required mixing times and ignition chemistry times can be controlled simultaneously. Fig. 19 compares the ignition delay and emissions as functions of the oxygen content for LTC with neat diesel fuel and dieselines. It is obvious that the ignition delay increases substantially with increases in the gasoline volume and the EGR rate. As a result, longer ignition duration is provided for the fuel/air mixing process. It is very interesting to observe that ultra-low NO*x* and smoke-free emissions are observed with 13.3% oxygen content for 40% gasoline/diesel blend-fueled LTC. Based on these findings, it can be concluded that the most important criteria for LTC is not oxygen content or EGR rate but the balance of the mixing timescale and the chemistry timescale [311,312]. LTC can be achieved with a higher oxygen content or a lower EGR rate by modulating the physical–chemical properties of the test fuel.

6. Fuel design and management for the control of SCCI combustion

6.1. *Strategies and methods of fuel design and management for SCCI combustion*

To date, it has been very difficult to expand HCCI or LTC to full engine load-speed operating ranges under existing technical methods and control strategies. To effectively utilize the advantages of HCCI and LTC, compound HCCI combustion based on mode transitions or mixture stratification was recently proposed. Compound HCCI combustion based on mode transition implies that the engine operates in HCCI mode or LTC mode at low, medium, and cruising loads and switches to SI mode or DICI mode at cold start, idle, and large to full loads [313–316]. The switch from HCCI to SI, including throttle action, can be achieved in less than ten cycles, but there is fluctuation from SI to HCCI mode that needs to be optimized [317]. Compound HCCI combustion based on mixture stratification is also known as stratified-charge compression-ignition (SCCI), premixed compression-ignition (PCI), partial HCCI (pHCCI), and premixed-charge compression-ignition (PCCI), among other names. In this combustion mode, the overall combustion history, in-cylinder stratification of the temperature field, mixture concentration, and fuel composition can be managed in real-time by modulating the

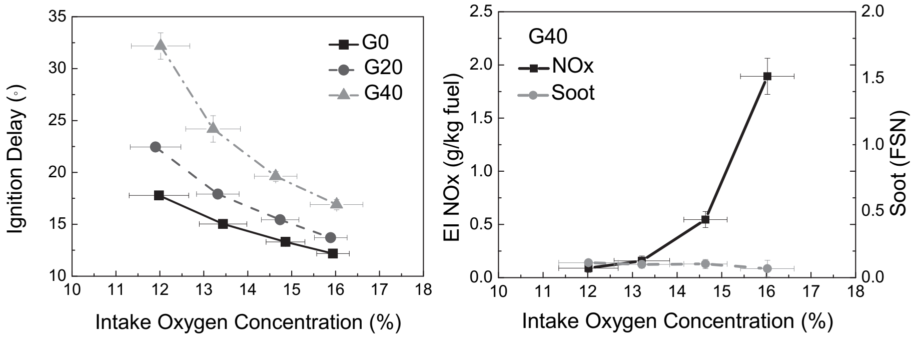

Fig. 19. Ignition delay and emissions of dieseline-fueled LTC as function of oxygen content [312].

controllable in-cylinder injection timing, spray mode, port fuel injection (PFI) combined with direct injection, fuel component design and management, and exhaust gas recirculation (EGR). As a result, high thermal efficiency with ultra-low emissions can be obtained throughout the overall engine operating ranges. For this combustion mode, there is no distinct borderline between HCCI combustion or LTC and traditional combustion. This mode features the advantages of both HCCI combustion or LTC and traditional combustion modes, and the combustion phasing and burn rate can be directly and flexibly controlled [318]. In fact, absolutely uniform fuel/air mixtures cannot be achieved, regardless of the mixture preparation methods, and some thermal or mixture inhomogeneities are always observed in real HCCI engines. In terms of "stratification", it is generally accepted that there are three aspects, i.e., temperature field stratification, mixture concentration stratification, and fuel composition stratification, that exist and are coupled in the cylinder.

Many researchers have noted that such small-scope and micro-level spatial stratifications have the potential to affect ignition timing and combustion rate. Johansson et al. [319–322] elaborated on the impact of concentration stratification and temperature stratification on HCCI combustion. The HCCI combustion progress was characterized by means of a high speed fuel tracer and PLIF combined with simultaneous chemiluminescence imaging. The authors found that in both spatial scopes and time histories, any minor variation and inhomogeneity in the temperature field and fuel concentration will affect the chemical reaction speed, and this influence will be amplified due to positive feedback. Sankaran et al. [323] and Bisetti et al. [324] reported analytical results of HCCI combustion investigations in the presence of charge stratification using the probability density function method. The results demonstrated that temperature and mixture stratification are effective means of controlling the start of combustion, reducing the abrupt pressure rise, and eliminating the auto-ignition of the end-gas at high loads. By means of a numerical simulation, Flowers et al. [325] also confirmed that the fuel/air mixture inhomogeneity exerts considerable impact on premixed HCCI combustion and emissions. As with the advantages of SCCI combustion, and due to the fact that some thermal or mixture inhomogeneities always exist in real HCCI engines and LTC engines [326], it is easy to achieve SCCI combustion through the modification of PFI gasoline engines or gasoline direct injection (GDI) engines. Furthermore, stratified methods can also be used in diesel fuel- and alternative fuel HCCI combustion and may be a good prospective direction in future.

Regarding mixture concentration stratification, Lee et al. [327,328] demonstrated that stratified mixture formation can be used to extend the operating range for SCCI combustion. Wang et al. [329] proposed a method for control of gasoline HCCI combustion phasing and extension of operating load by modulating the mixture formation using two-stage gasoline direct injection. Su et al. [330–341] developed a multi-pulse fuel injection technology used to control diesel fuel stratification by regulating injection pulse width, injection number, and dwell time between two neighboring pulses. As a result, with this mode, thermal efficiency can reach the same level as that of the conventional diesel combustion mode, while the NO*x* and smoke emissions can be simultaneously reduced on a large scale. Sjoberg et al. [332] created fuel stratification by injecting the main portion of the fuel during the intake stroke and the remainder during the compression stroke. It was found that partial fuel stratification may offer good potential for achieving a staged combustion event with a reduced pressure-rise rate and increasing the high-load limits. However, it should be noted that fuel stratification must be applied carefully, as too much stratification can quickly lead to unacceptable NO*x* emissions. Dahl et al. [333] verified that a stratified charge allows the maximum pressure-rise rate and ringing intensity to be reduced at the expense of increases in NO*x* and CO emissions. Berntsson et al. [334] confirmed that a stratified charge can influence combustion phasing and that increased stratification leads to an advanced CA50 timing. Choi et al. [335] investigated the effects on combustion stability of mixture stratification based on asymmetrical fuel injection to the intake port. Lu et al. [336] and Wang et al. [337] developed an SCCI combustion system based on a port fuel injection combined with in-cylinder direct injection. Aroonsrisopon et al. [338] employed two GDI injectors: one was used for generating a homogeneous mixture in the intake system, and the other was mounted directly into the side of the combustion chamber for variation of the degree of charge stratification. The results revealed that stratification yielded a tremendous improvement in IMEP and emissions at the lean limit of the operating range but not at the rich limit.

Compared to fuel stratification, it is very difficult to control fuel composition stratification and temperature stratification. Li et al. [339] proposed a fuel stratification concept using two different fuels or fuel components introduced separately into the cylinder through two independent inlet ports. This SCCI engine could operate with a very lean mixture or at high exhaust gas dilution under partial loads in order to reduce fuel consumption and NO*x* emissions. Inagaki et al. [340] created composition stratification with diesel fuel and iso-octane. The diesel fuel was directly injected into a cylinder during early timing, and iso-octane was injected into an intake port. Using this approach, moderate spatial inhomogeneities were created in-cylinder, not only in the local equivalence ratio but also in the research octane number. The experimental results revealed that the ignition timing of dual-fuel stratified combustion can be controlled by changing the ratio of the two fuels. Combustion proceeds very mildly because of the spatial stratification of ignitability in the cylinder even without EGR, thus preventing the entire mixture from igniting simultaneously.

Sjöberg and Dec [341,342] confirmed that thermal stratification has the potential to reduce the pressure-rise rate and allow increased output for the HCCI engine. The authors also pointed out that HCCI combustion demonstrates a high sensitivity to stratification when fueled with significant cool-flame chemistry. Stratification can also improve the low load combustion efficiency for conditions where bulk gas combustion is incomplete for all fuels, regardless of the low-temperature reaction intensity. Krasselt et al. [343,344] created thermal stratification and compositional stratification by applying different temperatures and reactant compositions from a split intake port of a four-valve engine. Argon was used as a diluent to achieve higher temperatures and stratify the in-cylinder temperature indirectly via stratification of the ratio of specific heats. Quantitative observations indicated that a ±20 °C temperature stratification, ±15% fuel concentration stratification, and ±5 air–fuel ratio stratification all similarly affected the combustion progress. Sankaran et al. [345] modeled the effect of various initial temperature distributions (including homogenous, hot core, and cold core) on auto-ignition in an HCCI-like environment. Lim et al. [346,347] performed fundamental research regarding the effect of thermal stratification in HCCI combustion of an n-heptane/iso-octane/air mixture in a rapid compression machine (RCM). The temperature stratification is created by the buoyancy effect in the combustion chamber of the RCM. It was also found that the combustion duration became shorter and the rate of pressure increase became smaller with the larger thermal distribution. The optical results revealed that with a small thermal distribution, ignition appeared nearly equally throughout the combustion chamber. Conversely, with a large thermal distribution, ignition occurred first in the upper part and then throughout the entire chamber. Sjoberg et al. [348] investigated the potential of in-cylinder thermal stratification for reducing the pressure-rise rate in HCCI engines and coupling between thermal stratification and

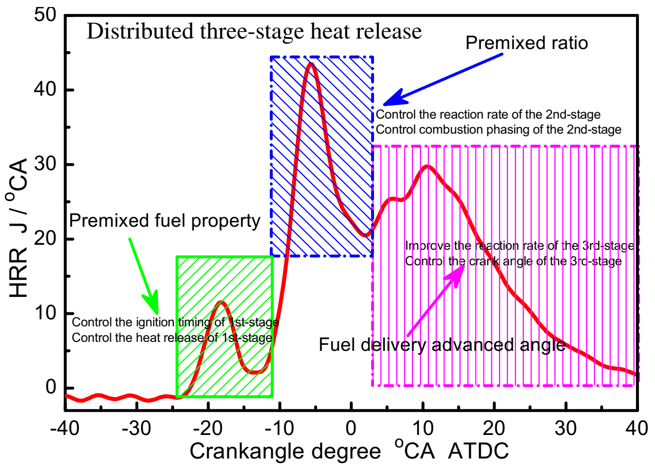

Fig. 20. Staged heat release and influence factors on SCCI combustion [350].

combustion-phasing retardation. With the appropriate stratification, even a stoichiometric charge can be combusted with a low pressure-rise rate, resulting in an output of 16-bar IMEP for naturally aspirated operation. The optimal charge-temperature distribution was found to depend both on the amount of fuel and the combustion phasing. For combustion phasing in the range of 7–10 °CA ATDC, a linear thermal distribution is optimal because it produces a near-linear pressure rise. Additionally, the total thermal width must be greater at higher fueling rates to avoid excessive pressure-rise rates. Sjoberg et al. [349] found that enhanced nature thermal stratification by increased heat transfer rates could substantially decrease the heat release rates and lower the knock intensity under certain conditions. Unfortunately, the higher heat losses associated with high air swirl decreased the IMEP.

Generally speaking, in order to achieve controllable ignition, a smooth heat release, maximum thermal efficiency, lower emissions, and wider engine load, moderate spatial and time-history inhomogeneities are necessary in the cylinder, and these include not only the air–fuel ratio and temperature field, but also the fuel composition. Fig. 20 displays a classical heat release curve for SCCI combustion. From the macroscopic characterization of this curve, it can be found that SCCI combustion exhibits a smoothly staged heat release. In this staged combustion, the ignition timing and peak value of the first-stage combustion have an important impact on the combustion phasing and the peak point of the second-stage combustion. The dominant factors of the first-stage reaction are the chemical properties and quantities of the premixed fuel. The second-stage combustion phasing and peak point have a crucial influence on the ignition timing of the third-stage combustion, maximum gas temperature, thermal efficiency, and knock intensity or pressure-rise rate. The crucial factors in the second-stage reaction are the premixed ratio (R_p) and the chemical properties and quantities of premixed fuel. The third-stage combustion dominates the overall combustion efficiency, engine thermal efficiency, and NO*x* and other emissions. The driving factor in this combustion is the main fuel injection timing.

If the combustion phasing and peak value of each stage of the reaction can be flexibly controlled using mixture concentration stratification, temperature stratification, and composition stratification, then the maximum thermal efficiency, minimum NO*x* emissions, and expanded engine load may be obtained. This target is impossible to achieve using only fuel design or fuel injection strategies, but it may be reachable using a combination of these two methods. This is the fundamental principle of fuel design and management, as shown in Fig. 21.

According to the inherent defects of the HCCI combustion process, the fundamental principles of fuel design and management can be described as follows.

(1) Design fuel physical–chemical properties and molecular components in real-time according to the operating ranges and selected test fuels.
(2) Create appropriate fuel concentration stratification using fuel supply strategies (for example, port fuel injection combined with in-cylinder direct injection, multi-hole in-cylinder injection and controllable injection timing, injection mode, and split injections).
(3) Select test fuels with opposing chemical properties to serve as port injected fuels and direct-injected fuels and modulate the spatial local fuel/air composition.

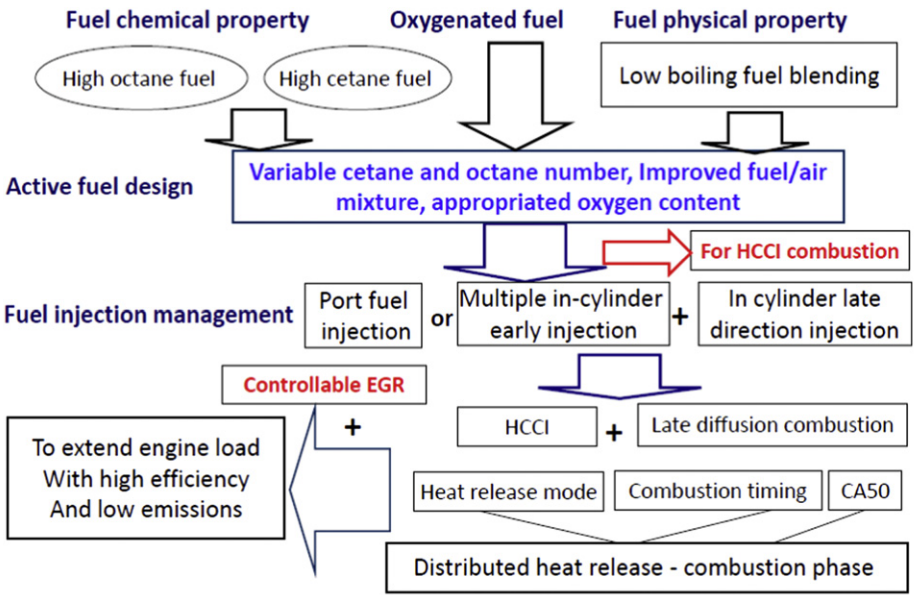

Fig. 21. Fundamental principles of fuel design and management for SCCI combustion.

(4) Use controllable EGR as an effective way to depress the combustion rate and control the maximum combustion temperature. By using this strategy, the onset and heat release of the low-temperature reaction, ignition timing and oxidation extent of the second-stage reaction, and the heat release mode and ignition timing of the third-stage can be modulated in a flexible manner.

6.2. *Effect of stratification on SCCI combustion with diesel-like fuels*

Partial fuel stratification shows potential for achieving a staged combustion event with reduced pressure-rise rates, and thus, partial fuel stratification has the potential to increase high-load limits for HCCI/SCCI operation. Sjoberg et al. created fuel stratification by injecting the main portion of the fuel during the intake stroke and the remainder during the compression stroke [332]. The results revealed that the hot ignition timing showed sufficient sensitivity to the local equivalence ratio when the fuel exhibited low-temperature heat release. Conversely, for a single-stage ignition fuel, the timing of the "hot" ignition is relatively insensitive to the local equivalence ratio, and this renders partial fuel stratification ineffective for creating a staged combustion event. Dec et al. investigated the relative magnitude of various factors on SCCI combustion phasing when fueled with iso-octane, commercial gasoline, and PRF80. These factors included fuel auto-ignition chemistry, thermodynamic properties, combustion duration, wall temperatures, residuals, and heating/cooling during induction [351]. It can be concluded that fuels with significant cool-flame chemistry require immediate and substantial compensation as the fueling rate is altered and additional compensation as the wall temperatures equilibrate.

In-cylinder multiple early injection or port fuel injection combined with direct injection are important methods used to achieve SCCI combustion. Specifically, for port fuel injection or in-cylinder early injection of a significant cool-flame chemistry fuel, mixture concentration variation offers an effective strategy for the control of SCCI combustion phasing because the amount of low-temperature heat released is proportional to the local equivalence ratio. As a result, the combustion phasing may be managed within one cycle by altering the injection timing to control the mixture stratification. In addition, fuel stratification can also be used to adjust the burn duration using various fuel injection strategies. This means that partial fuel stratification can be used to create a staged auto-ignition event, thus extending the burn duration and lowering the pressure-rise rate [352].

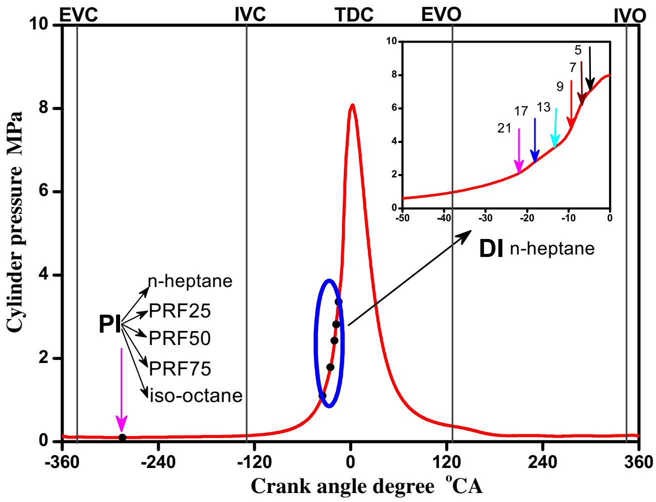

Fig. 22. Stratifications of n-heptane SCCI combustion [350].

Stratification, therefore, can be used to depress the maximum pressure-rise rate and extend the engine operating load range at the expense of the NO*x* and CO emissions. It should be noted that the indicated thermal efficiency of the SCCI combustion is lower than that of traditional DICI engines and neat HCCI engines due to the fact that the combustion phasing, heat release mode, and other combustion parameters are not optimized. For these reasons, the problem of how to achieve the lowest NO*x* emissions and highest thermal efficiency by modulation of the stratification and fuel injection timing is a core issue in SCCI combustion. Fig. 22 shows the n-heptane SCCI combustion system with port fuel injection of the PRF mixture. By altering the iso-octane/n-heptane proportions of the premixed fuel, the mixture composition and temperature stratification are created in the cylinder due to the LTR and HTR of premixed n-heptane. Furthermore, by adjusting the injection timing, the fuel concentration stratification may be altered.

Fig. 23 illustrates the effects of premixed fuel properties and injection timing on SCCI combustion. Specifically, Fig. 23a shows the influence of fuel delivery timing on the heat release rate at a fixed overall equivalence ratio and premixed ratio. It is obvious that the n-heptane delivery timing has a profound influence on the ignition timing and the peak values and their crank angle in the third-stage combustion, but it has only a moderate effect on the first- and second-stage combustion. When the n-heptane delivery advance angle is delayed, the peak values, the maximum in-cylinder pressure, and the combustion temperature all drop. As a result, the CA50 is delayed substantially and the burn duration is prolonged slightly. This has the potential to depress NO*x* emissions but leads to a deterioration of fuel efficiency and an increase in other emissions. The conclusion is that the in-cylinder fuel delivery advance angle plays an important role in the engine-indicated thermal efficiency, and the earlier fuel delivery angle has a positive effect on the indicated thermal efficiency. However, an excessively advanced fuel delivery angle will lead to a sharp increase in NO*x* emissions.

Fig. 23b displays the effects of premixed fuel properties on the heat release rate (HRR) at a fixed overall equivalence ratio, premixed ratio, and fuel delivery advance angle. In addition to port fuel injection of iso-octane, the overall heat release rate displays three-stage combustion. The premixed fuel properties have significant effects on the first- and second-stage combustion phasing and peak points but have negligible effects on the third-stage peak point and its diffusion combustion. With the delaying of the first- and second-stage combustion, the overall heat release centers on the top dead center position, which has a positive effect on thermal efficiency. This also means that the LTR and HTR of SCCI combustion can be changed by altering the premixed fuel properties. Contrast to the other combustion behavior, in the case of iso-octane port fuel injection, the n-heptane ignites the premixed iso-octane. The heat release shows single-stage combustion behavior, and the ignition timing of main combustion occurs much later than that of the aforementioned SCCI combustion

By optimizing the premixed ratio, premixed fuel properties, and n-heptane injection timing, controllable ignition timing and smooth heat release were obtained. Additionally, partial burn or misfire at the lean limit, as well as knock combustion, was eliminated to some extent, and the operating range was expanded to the full engine speed-load range. In addition, Fig. 24 shows that the NO*x* emissions of SCCI combustion are significantly lower than that of the tradition diesel engine, and the thermal efficiencies are higher than DICI and comparable to that of HCCI combustion.

6.3. *Effect of stratification on SCCI combustion with gasoline-like fuels*

It is well known that the HCCI combustion is dominated by the chemical kinetics of the fuel/air mixture. This process is strongly

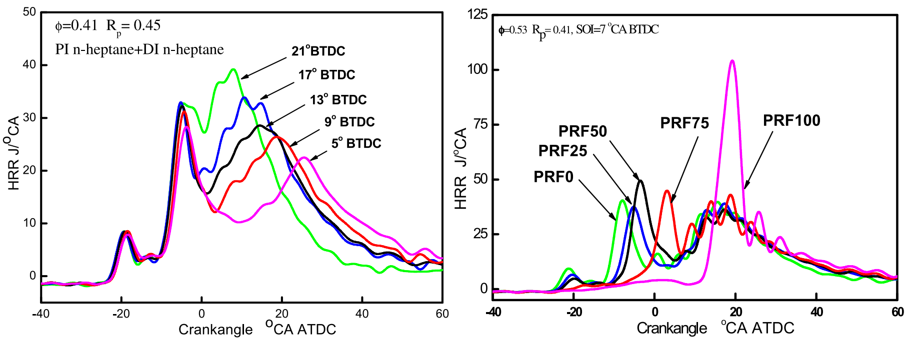

Fig. 23. Effect of premixed fuel property and n-heptane injection timing on SCCI combustion.

temperature dependent and is also influenced by fuel concentrations and fuel molecular structure. Gasoline fuel features a high octane number and long branched-chain structure and does not tend to react with air at low to intermediate temperature ranges. Additionally, moderately active radicals are observed during the compression stroke, which cannot trigger the combustion event until the critical decomposition temperature is achieved. Earlier gasoline HCCI investigations used a high degree of intake charge preheating, up to 300 °C, so that the compression temperature near TDC reached the fuel decomposition temperature in order to produce stable HCCI combustion [353]. However, this method cannot be practically applied due to the problem of large heat inertia. Another means used to achieve gasoline HCCI combustion is the increase of the compression ratio up to the required temperature and pressure for auto-ignition. Additionally, the use of large amounts of burned gas trapping [354] or exhaust gas re-breathing [355] via variable valve timing and/or lift (VVT/VVL) are other successful and practical approaches for gasoline HCCI combustion. In this manner, auto-ignited combustion can begin at the right time and proceed without causing runaway heat release rate.

In recent years, much effort has been put into gasoline HCCI investigation, with specific attention paid to the control of ignition phasing and combustion rate, the mode transition between SI and HCCI, expansion of the engine speed-load range, and combustion stability at operating limits. Wang et al. [356] introduced a second fuel injection during the compression stroke, by which a stratified charge can be formed and the mixture can be cooled; then, the HCCI ignition timing may be controlled by tuning the mixture concentration and temperature. Song et al. [357] further elucidated the fuel preprocessing (fuel-reforming, fuel recompression reaction) mechanism of pilot-injected fuel during negative valve overlap. It was found that exothermic reactions, reforming reactions or fuel pyrolysis, and charge cooling can affect low load HCCI operation with high residual mass fractions and low equivalence ratios.

In essence, HCCI combustion is the chemical reaction of fuel/air mixtures, which exhibit different reaction pathways and reaction rates for various hydrocarbon fuels under practical engine operating conditions. High cetane number fuels such as n-heptane feature a low-temperature reaction, negative temperature coefficient, and high-temperature reaction. Certain high octane number fuels such as iso-octane also exhibit a three-stage heat release, including cool flame, extra heat release, and final ignition stages [219]. Therefore, to control gasoline HCCI combustion, an efficient approach is to modulate the concentration of active radicals and their distribution during the fuel/air mixture compression process in order to alter the reaction pathways [93]. Song et al. [358] verified that the extent of the recompression reaction is limited by chemical kinetics rather than thermodynamics, and that residual oxygen during NVO acts as a key species for the extent and speciation of the recompression reaction.

In fact, the modern HCCI concept originates from that of active thermal atmosphere combustion (ATAC), which was proposed by Onishi et al. [1]. Gasoline self-ignition, assisted by the preheating and pre-reaction of active radicals in the fuel/air mixture, was achieved by high levels of residual gas at part-throttle operation. The fuel consumption and exhaust emissions of two-stroke spark-ignition engines are remarkably improved with ATAC, whereas noise and vibration are reduced. Due to the substantial advantages of ATAC, Ishibashi et al. [359–361] applied it to practical use in some motorcycle engines and referred to it as activated radical (AR) combustion. For two-stroke SI engines, direct fuel injection allows

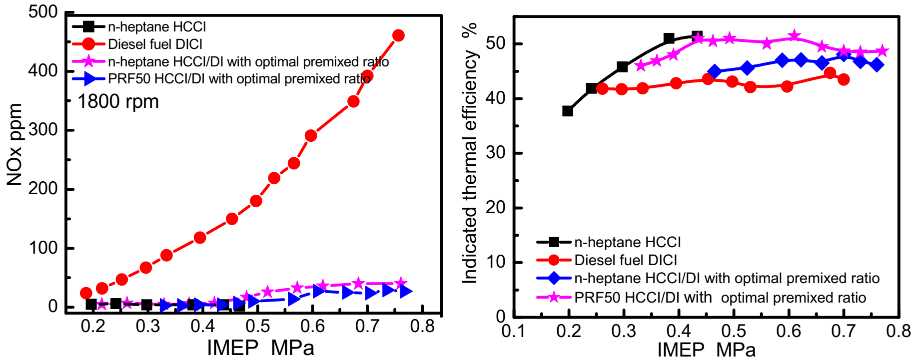

Fig. 24. Comparison of NO*x* emissions and thermal efficiencies among HCCI, DICI, and SCCI.

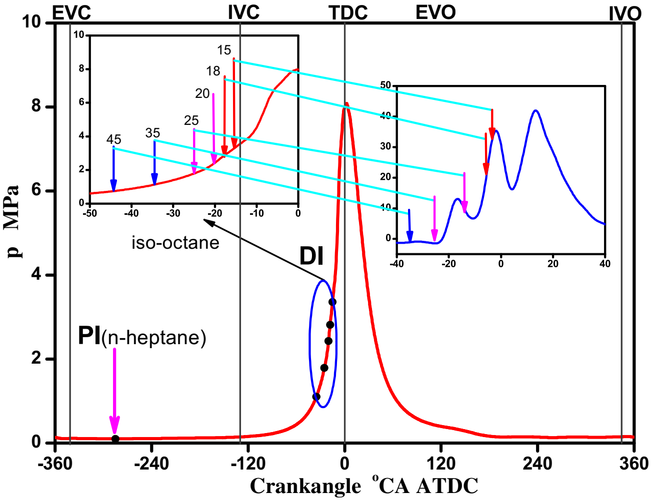

Fig. 25. Fuel strategy of iso-octane ATAC assisted by premixing of n-heptane [371].

avoidance of fuel loss from the exhaust port. For this reason, Gentil et al. [362–364] incorporated ATAC into GDI two-stroke engines, utilizing the thermal energy of residual gas to promote the combustion of fresh gas. ATAC leads to very good combustion stability, good fuel economy, and low exhaust emissions of unburned hydrocarbons. Iida et al. [365,366] obtained fundamental knowledge regarding the control of the auto-ignition and combustion characteristics in an ATAC engine fueled with methanol, ethanol, and other light-molecule fuels. It was found that the ATAC auto-ignition temperature and combustion duration did not depend on the delivery ratio and equivalence ratio but were rather determined by the fuel properties. Iijim et al. [367] compared ATAC and HCCI in a two-stroke engine. The results indicated that the main differences between ATAC and HCCI combustion were found in their different low-temperature oxidation reaction characteristics. Cool-flame reactions are less likely to occur in ATAC as compared with HCCI combustion. Recently, Lu et al. evaluated the effect on ATAC induced by the port fuel injection of n-heptane in diesel-fueled and biodiesel-fueled engine combustion and emissions [368,369]. Ogawa selected methanol as an inhibitor in order to depress HCCI combustion with port fuel injection of n-heptane, PRF25, and PRF50 [370]. Although the major purpose of their work was to depress the low-temperature oxidation and high-temperature oxidation processes by adding methanol so as to prevent knock combustion, it was found that the ignition and combustion of methanol are completed under the action of thermal energy and active radicals released by premixed fuels.

It is well known that the LTR, NTC, and HTR occur sequentially in the n-heptane/air mixture during the compression processes. In addition, the LTR is characterized by some amount of active radicals and a small amount of heat release, the NTC features a lower reaction speed and plenty of H_2O_2, but the HTR displays the main heat release. Based on this behavior, an active thermal atmosphere environment is created and can be adjusted by changing the n-heptane quantities. The iso-octane is directly injected into the combustion chamber near TDC, and ignition may be triggered by the thermal energy and radicals. This combustion mode displays slightly different behavior than does the SCCI combustion in Section 6.2. In this combustion process, the iso-octane ignites and burns after the n-heptane, and thus this combustion phenomenon is also called as dual-fuel sequential combustion (DFSC) [371]. Fig. 25 shows the experimental results for a system of iso-octane ATAC assisted by premixed n-heptane.

Fig. 26 compares combustion and emissions at various premixed ratios with the overall equivalence ratio held at constant. With a premixed ratio at 0.3, the n-heptane equivalence ratio is approximately 0.11, and the iso-octane ignition and combustion are dominated by active radicals produced from the incomplete HTR. When the fuel delivery angle is at 25 °CA BTDC, the diffusion burn occurs near TDC, which leads to intense heat release and considerable NO*x* emissions as well as a high thermal efficiency. With the increase of the premixed ratio to 0.5–0.6, the heat release and active radicals that are produced from the HTR trigger the iso-octane ignition and combustion. Despite the earlier ignition timing of the third-stage combustion, the burn speeds are

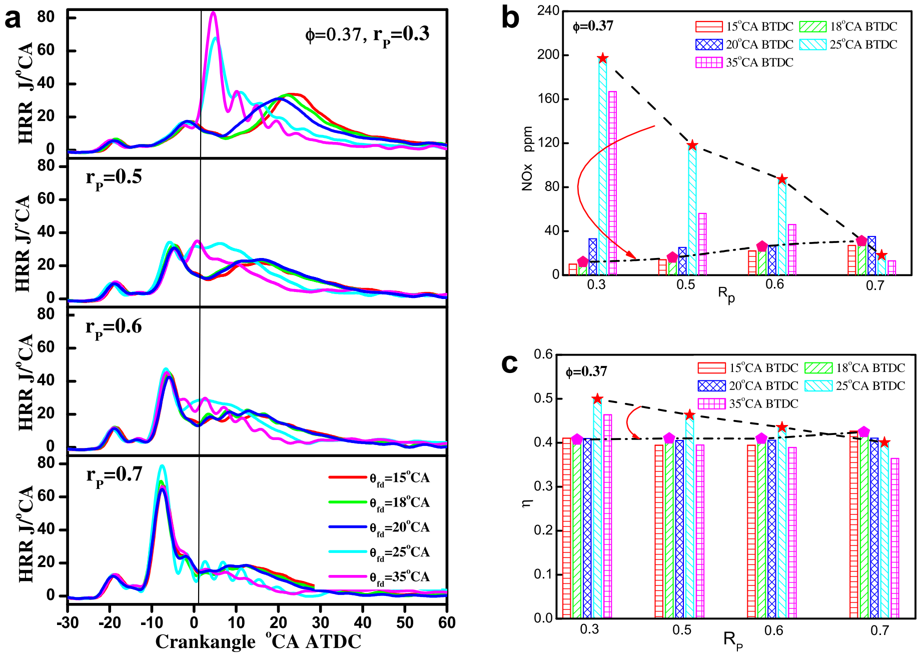

Fig. 26. Effects of premixed ratio and n-heptane injection timing on combustion, emissions, and thermal efficiency of iso-octane ATAC [371].

depressed to a low level and are extended into the expansion stroke. As a result, both the NO*x* emissions and thermal efficiency are decreased. As the premixed ratio further increases up to 0.7, the heat release during the completed HTR dominates the iso-octane ignition. Despite the improvement in the ignition, the combustion rate is further decreased due to the lean iso-octane/air mixture. As a result, both the NO*x* and thermal efficiency reach levels that are too low.

Based on the attainable degree of n-heptane oxidation during the compression process as well as the quenching effect and charge cooling of the directly injected iso-octane, iso-octane ignition and combustion may be classified into three modes: thermal atmosphere combustion, active atmosphere combustion, and active thermal atmosphere combustion. The combustion mode mainly depends on the n-heptane equivalence ratio, iso-octane equivalence ratio, and fuel delivery advance angle of iso-octane.

Regardless of the iso-octane equivalence ratio and the delivery advance angle, iso-octane ignition and combustion is dominated by active atmospheres for lower n-heptane equivalence ratios and is dominated by active thermal atmospheres for medium n-heptane equivalence ratios. With a large n-heptane equivalence ratio, iso-octane ignition is primarily triggered due to thermal atmospheres, except at conditions of larger iso-octane equivalence ratios and earlier fuel delivery angles.

For low to medium iso-octane equivalence ratios, regardless of fuel delivery advance angle, iso-octane ignition is dominated by thermal atmospheres produced by high n-heptane equivalence ratios, by active thermal atmospheres at medium n-heptane equivalence ratios, and by active atmospheres with small n-heptane equivalence ratios. For large iso-octane equivalence ratios, ignition and combustion are dominated by active thermal atmospheres or active atmospheres.

The ignition timing of iso-octane ATAC assisted by the n-heptane two-stage reaction can be flexibly controlled. For the ATAC dominated by the thermal and active thermal atmospheres, ignition delay is only dominated by the n-heptane equivalence ratio. For the ATAC dominated by active atmospheres, ignition-timing delays are affected to a small degree by the notable charge cooling that occurs as the iso-octane equivalence ratio increases [371,372].

Due to the significantly effect of active radicals on ignition and combustion, Splitter et al. have proposed a new combustion concept, radical controlled compression ignition (RCCI) Combustion [373]. Unlike dual-fuel combustion technology, RCCI operates with a single fuel stock (gasoline) as the basis for both high- and low-reactivity fuels. The fuel supply system consists of port fuel injection of gasoline and direct injection of the same gasoline doped with a small volume percent addition of DTBP. With 1.75% DTBP by volume added to only the direct-injected fuel (which accounts for approximately 0.2% of the total fuel), it was found that the additized gasoline behaved similarly to diesel fuel, allowing for efficient RCCI combustion. The results demonstrate that a very small percentage of an appropriate additive can be used to establish a sufficiently large reactivity gradient to match the performance of a dual-fuel strategy when operated in the RCCI combustion regime.

6.4. *SCCI combustion of gasoline-diesel dual-fuel and blends*

The products refined from crude petroleum oil, gasoline and diesel, are two basic fuels that have been widely utilized as main fuels since the invention of the internal combustion engine. Unfortunately, there are many theoretical and practical obstacles to HCCI combustion fueled with diesel fuel or gasoline. Gasoline, which has high volatility but low ignitability, is generally produced as a high octane number fuel. Diesel fuel, which has poor volatility but excellent ignitability, is generally produced as a high cetane number fuel. A variety of physical and chemical control methods that can contribute to combustion control have been examined, including fuel injection strategies, fuel blending, fuel additives, and fuel reforming. However, the methodology with the best prospects involves investigation of the HCCI combustion behavior using dual-fuel or mixtures of gasoline and diesel, two fuels with opposite but complementary properties. In fact, roughly ten years ago, there was some research on quasi-HCCI combustion with gasoline/diesel dual-fuel systems. Recently, Yao et al. investigated methanol/diesel dual-fuel combustion characteristics [374], and Lu et al. carried out an experimental study on ethanol/biodiesel and propanol/biodiesel dual-fuel combustion and emissions [375,376]. It should be noted that these combustion behaviors are commonly characterized by the injected diesel fuel or biodiesel near TDC that is used to trigger and control the ignition of the overall fuel/air mixtures. It should be pointed out is that, due to the shorter ignition delay of injected diesel or biodiesel fuel and the homogenous fuel/air mixture that has been formed before diesel is injected into the cylinder, moderate stratifications are created in the cylinder, affecting not only the local equivalence ratio but also the composition of the mixture. Accordingly, this dual-fuel combustion system is known as qHCCI, pHCCI, PCI, or SCCI, according to different authors.

Can et al. investigated gasoline/diesel dual-fuel combustion and emissions with a gasoline premixed ratio between 10% and 30%. HCCI combustion and diffusion combustion were observed in one combustion event. Furthermore, the NO*x* and soot trade-off characteristics were altered, and improvements in both NO*x* and soot emissions were observed simultaneously, with decreases of up to 16% and 65%, respectively [377]. Kim et al. compared SCCI combustion and emissions for premixed gasoline, diesel, and n-heptane with the direct injection of diesel fuel [378–381]. The results indicated that the combustion event exhibits one-stage heat release with premixing of gasoline, but premixed diesel fuel was accompanied by

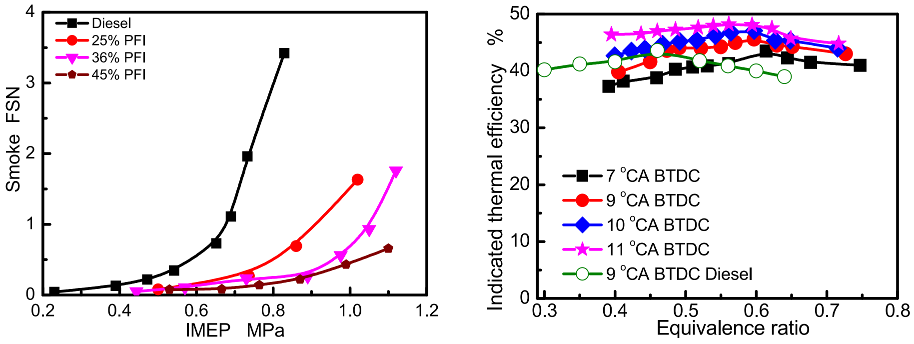

Fig. 27. NO*x*–smoke emissions and indicated thermal efficiency of gasoline/diesel dual-fuel combustion.

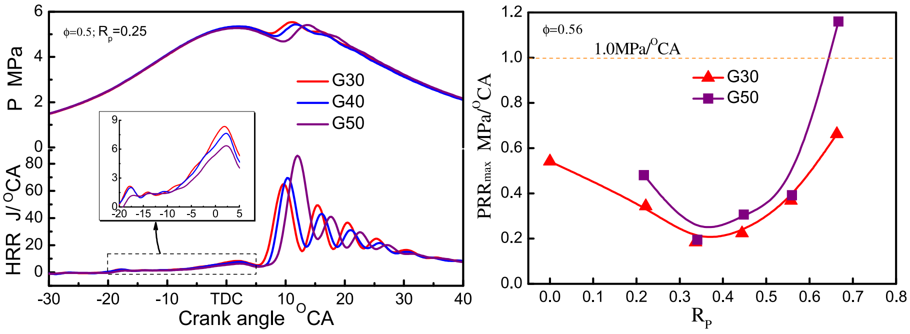

Fig. 28. Combustion characteristics and pressure-rise rate of dieseline SCCI with two-stage fuel supply.

a cool flame prior to the combustion of the directly injected diesel fuel. NO*x* emissions in the partial HCCI engine with premixed gasoline fuel decreased linearly with increases in premixed ratio. For premixed diesel fuel, NO*x* emissions were increased at high intake temperature and high premixed ratio conditions. The ignition and combustion mechanisms for premixed high cetane number fuels are unlike those of premixed gasoline. With premixed diesel fuel and n-heptane, the combustion event exhibits earlier ignition timing and a sharp combustion rate. Cooled EGR can be used to control the ignition and burn rate [382]. Kokjohn et al. hypothesized that varying the in-cylinder fuel reactivity using the port fuel injection of gasoline and the direct injection of diesel fuel could be used for combustion phasing control at both high and low engine loads, and also to control the rate of pressure-rise [383]. It was found that the optimal fuel reactivity was decreased as load increased. The experimental results confirmed that an extension of the PCCI operating regime is possible when optimized fuel blends are used. At the 11-bar operating point, NO*x* and soot levels were ~0.01 g/kW-hr and ~0.008 g/kW-hr, respectively. This means that the US 2010 heavy duty emissions regulations can be easily met without after-treatment while achieving 50% thermal efficiency. Recent results have revealed that a maximum thermal efficiency of 53% can be achieved with optimized fuel design and management [384,385]. Gasoline-diesel dual-fuel SCCI combustion addresses many of the problems of high efficiency premixed combustion, e.g., lack of combustion phasing control, high PRR, and load limitations. Therefore, this represents a promising method with which to meet future emissions regulations in-cylinder without the use of expensive after-treatment systems, increasing internal combustion engine efficiency.

Fig. 27 displays the NO*x*/smoke emissions and indicated thermal efficiency of gasoline/diesel dual-fuel combustion from experiments conducted on a single-cylinder naturally aspirated light-duty diesel engine. It is clear that both the NO*x* and smoke opacity were improved significantly with an increase in the premixed ratio of the gasoline. In addition, the thermal efficiency with earlier direct injection timing reached a high level over all engine load ranges. However, it should be noted that the pressure-rise rate increased sharply for large premixed ratios.

In addition to gasoline/diesel dual-fuel SCCI combustion, HCCI and LTC fueled with gasoline/diesel blends have also been investigated by many researchers, as covered in Sections 3.3.3 and 5.3. However, dieseline HCCI combustion has still not broken through the limitations of narrow operating load, uncontrollable ignition, and combustion rate. To address these problems, SCCI combustion using "dieseline" can be used to expand the engine load. Figs. 28 and 29 compare the combustion characteristics, pressure-rise rate, and NO*x*–smoke emissions for 30%, 40%, and 50% gasoline/diesel blends (G30, G40, G50 respectively) using PFI combined with direct injection.

Given the lower boiling point, smaller viscosity, improved volatility, and reduced cetane number of dieseline as compared to neat diesel fuel, dieseline requires a reduced physical mixing timescale but an extended mixture ignition timescale. The overall combustion event of dieseline PFI plus DICI appears as three-stage combustion, including a weak cool-flame reaction, a moderate high-temperature reaction, and intense diffusion combustion, as shown in Fig. 28. With an increase in the gasoline proportion in blends, the heat release onset is delayed and the peak values are decrease both in the first- and second-stage reactions, but increase clearly in the third-stage. However, it is very interesting to note that the pressure-rise rate is maintained at a low level over a wide range of premixed ratios, only increasing to higher rates at large premixed ratios.

In Fig. 29, it can be seen that the NO*x* emissions of dieseline SCCI with a two-stage fuel supply were significantly decreased. Regardless of the gasoline proportion used in blends, NO*x* emissions were improved up to 85% at premixed ratios of 50%–60%, whereas the smoke emissions increased moderately but still

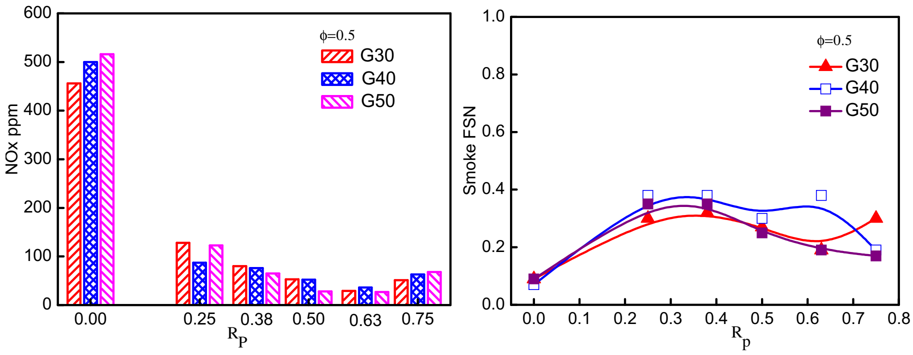

Fig. 29. Effect of premixed ratio on NO*x* and smoke emissions of dieseline SCCI with two-stage fuel supply.

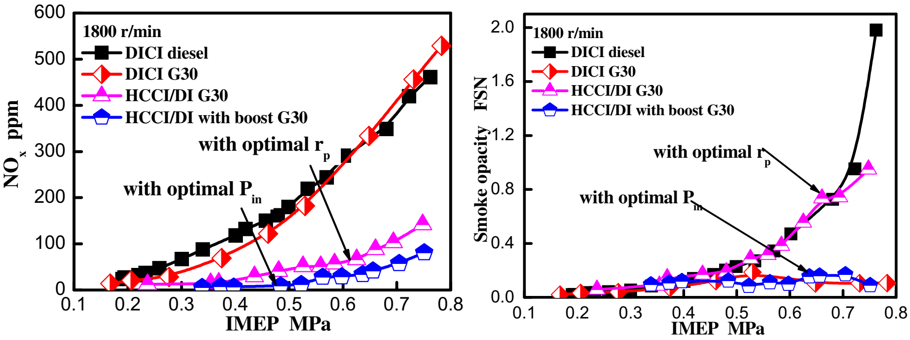

Fig. 30. Comparison of NO*x* and smoke emissions for different strategies.

remained at relatively low levels. Moreover, NO*x*–smoke emissions show little sensitivity to the gasoline ratio in the range of 30%–50%.

Intake charge boosting can be used to further improve the smoke emissions. Fig. 30 compares the smoke and NO*x* emissions of 30% gasoline/diesel blend fuel (G30) with different methods, including traditional DICI and SCCI combustion with a two-stage fuel supply, and SCCI combustion with a two-stage fuel supply supplemented with intake boosting. In the case of the original diesel engine, DICI G30 demonstrates ultra-low smoke emissions due to the homogenous mixture formed before ignition occurs. The NO*x* emissions show negligible improvement over those of neat diesel at low to medium loads, but are increased slightly at high engine loads due to the excessively fast combustion rate. With the two-stage fuel supply, NO*x* emissions were reduced to a very low level due to the controlled combustion rate, but smoke emissions remained at a high level due to a locally rich fuel/air mixture and shorter ignition delay in these areas. When supplemented with intake charge boosting, both the NO*x* and smoke emissions were reduced to ultra-low levels.

6.5. *Partially premixed compression ignition of gasoline and diesel fuel*

Recently, many researchers focused on partially premixed compression ignition (PCI or PPCI) combustion [386,387], which is very similar to SCCI combustion. The target of PPCI is to achieve a separation between the end of the injection and the start of the combustion. There are many ways to accomplish the separation between end of injection and start of combustion: inject fuel very early in the cycle, decrease the compression ratio, use a large amount of EGR and decrease the cetane number of the fuels. In general, PPCI requires high EGR levels and injection timings sufficiently early or late to extend the ignition delay so that air and fuel mix extensively prior to combustion. Noehre et al implemented diesel PCCI at high load and by using 70% of EGR and a compression ratio of 12:1, it was able to achieve the separation between injection and combustion event at 15 bar BMEP; low NO*x* and low soot were achieved but unfortunately the efficiency was unacceptably low [278]. Since the shorter ignition delay, diesel fuelled PPCI operating range was proved to be limited [388]. The short ignition delay of conventional diesel fuel requires high fuel injection pressures to achieve adequate premixing along with high levels of EGR to achieve low NO*x* emissions [227].

While, the most effective way to run this combustion mode is using high octane number fuel. To improve the high load operational PCCI widow, in 2006 Kalghatgi et al researched the partially pre-mixed combustion by dual injection using gasoline and diesel fuels with cetane numbers from 30 to 54 [389,390]. As result, one of the operating points reached with gasoline (RON95) with double injection had mean IMEP of 15.95 bar with lower smoke and NO*x* emission. At the same operating conditions, to get such low level of smoke with diesel fuel, IMEP has to be below 6.5 bar.

Hildingsson et al evaluated the effect of octane number on PCI combustion. The gasoline fuels with octane numbers of 91, 84, 78, and 72 were compared at a low load/low speed condition in SOI sweeps as well as at a higher load and speeds in EGR sweeps [391]. Moreover, Manente et al compared the PPCI combustion with diesel fuel, ethanol, and gasoline at 14.80 bar gross IMEP with 25% of EGR. Due to the longer ignition delay, high ON fuels have lower NO*x* and soot production, as compared to Diesel, because of the lower heterogeneity at the moment of the ignition [392]. Furthermore, the effects of fuel properties on the performance and emissions of an engine running in partially premixed combustion mode were investigated using nine test fuels RON from 69 to 99 developed in the gasoline boiling point range. The fuels covered a broad range of ignition quality and fuel chemistry. Gross indicated efficiencies higher than 50% can be achieved. Fuels with an Octane Number below 90 and higher than 69, at 1300 rpm, have a gross indicated efficiency between 55 and 57% [393].

Through gasoline PPCI combustion can be extended to higher engine load, while it should be noticed that pressure oscillations after the combustion event are able to enhance the heat transfer thus resulting in higher fuel consumption. In addition, there are some problems of this combustion mode under lower engine load. A combination of increased fuel stratification, intake pressure and temperature is required to achieve low emissions and acceptable combustion stability. A moderate reduction in octane rating from the RON95 value used would reduce the requirement for raised intake pressure and temperature due to an increase of low-temperature heat release and reduction of ignition delay [394].

7. Summaries and future research directions

In order to break through the emission and energy utilization limitations that exist with traditional internal combustion engines, meet stringent emission regulations, and significantly reduce carbon dioxide emissions on a large scale, one possible solution is to integrate advanced compression-ignition combustion modes into existing commercial engines. Next-generation advanced combustion modes, including homogeneous-charge compression-ignition, low-temperature combustion, and stratified-charge compression-ignition, commonly feature extremely low NO*x* emissions and nearly smoke-free exhaust while simultaneously maintaining diesel-like thermal efficiency. Until now, advanced combustion modes have suffered from uncontrollable ignition and combustion rates, narrow operating load ranges, high levels of CO and HC emissions, and difficulty in cold start and mode transitions. As one of the unique operating principles of these combustion modes is that the ignition and combustion are mainly dominated by the chemical kinetics of fuel/air/residual gas mixtures and are only moderately influenced by turbulence and mixing, fuel design and management has become an important manner in which to resolve these difficulties and dilemmas.

7.1. HCCI combustion

A fundamental principle of the fuel design concept for HCCI control is that by modulating the fuel/air reaction pathway, the reaction rate, intermediate species, and concentrations through reforming of the fuel composition and components, the major combustion parameters, including reaction onset, cumulative heat release, and CA50, can be flexibly controlled during the low-temperature reaction. As a result, the pressure- and temperature-time histories and combustion phasing of the HTR can be controlled. The major strategies of fuel design include the use of fuel additives, blending, dual-fuel systems, and optimization of the fuel blending proportions in real-time.

The use of fuel additives and fuel blending has the capacity to expand the HCCI operating ranges to some extent; however, even fixed fuel additives or blends with given physical–chemical properties cannot expand HCCI operation to the full operating range. From the perspective of ignition control and load extension, the ideal strategy is to select two fuels with entirely opposing chemical properties and to control their proportions in real-time while considering the combustion characteristics, emission levels, and engine operating conditions. This is the principle of real-time fuel design.

Real-time fuel proportion optimization can flexibly control ignition timing, broaden the HCCI combustion operational range, improve cold start, and increase engine thermal efficiency. Furthermore, when combined with a closed-loop control strategy based on detailed combustion characteristics from the previous cycle, a real-time fuel design strategy can achieve rapid transient response within one cycle. The HCCI operational range can also be elevated to 60%–70% of the full load.

Future research directions in HCCI combustion: Some key scientific problems remain to be investigated for HCCI combustion based on the fuel design strategy. These problems include defining the characteristic parameters of the fuel index that are suitable for HCCI combustion, finding a group of fuels with opposite chemical properties in both LTR and HTR and with different hot ignition temperatures for cycle-to-cycle control of the combustion process, developing advanced control methods and exploring new combustion sensors, investigating ignition stability and emissions formation under cold start, mode transition, lean-burn limit, and rich-burn limit, among other conditions.

7.2. Low-temperature combustion

By utilizing high-pressure and multiple-stage fuel injection as well as heavy EGR or low oxygen content, low-temperature combustion of diesel-like fuels with poor volatility but excellent ignitability was achieved with local and global temperatures below the critical temperature for NO*x* and soot formation. The key goal of low-temperature combustion strategies is the harmonic combination of fuel injection strategy, in-cylinder flow field, and the amount of EGR. For LTC, high-pressure and multiple-stage injection combined with intensive in-cylinder turbulence was used to reduce the required timescale (τ_1) for mixture formation. A high level of EGR or lower oxygen content was used to extend the chemical timescale (τ_2) of the mixture ignition chemistry. Low temperature combustion is produced as long as $\tau_1 < \tau_2$ for the local mixture but $\tau_1 >> \tau_2$ for the global mixture. For diesel fuels, EGR rates higher than 60% (oxygen content less than 10%) and an ignition delay of 1.2–1.5 ms are sufficient to achieve low-temperature combustion. In low-temperature combustion mode, NO*x* and soot emissions are decreased at the expense of increased HC and CO emissions, thus leading to a slight reduction in thermal efficiency.

LTC may be further optimized by adjustment of physico-chemical properties and fuel components. A moderately reduced fuel cetane number extends τ_2 to some extent, and reduced viscosity and distillation temperature reduces τ_1, whereas the oxygen content in the fuel molecule has the potential to depress soot formation. Therefore, low-temperature combustion using oxygenated fuels such as DME and biodiesel can be achieved at a relatively low EGR rates with improved combustion stability and cycle-to-cycle variation. Moreover, gasoline/diesel blended fuels are suitable for low-temperature combustion. It is interesting to note that ultra-low NO*x* emissions and smoke-free exhaust are observed with 13.3% oxygen content for 40% gasoline/diesel blend-fueled LTC. This means that LTC can be achieved with a higher oxygen content or lower EGR rate by modulating the physico-chemical properties of the test fuel.

Future research directions in low-temperature combustion: Low-temperature combustion is one prospective combustion technology for achievement of the future stringent emissions regulations (EURO 6 and above). However, research in this area is still limited, and major problems remain to be solved, including in-cylinder fuel/air mixing control at full engine operational range, harmonic control of fuel properties, injection strategies, in-cylinder swirl, and EGR, the influence of EGR and fuel composition on ignition delay, pollutant formation and their evolution at high EGR rate or low oxygen content conditions, and pathways towards maximum thermal efficiency.

7.3. SCCI combustion

Due to the current difficulty of realizing full-range HCCI combustion or low-temperature combustion, an alternative combustion mode, stratified HCCI combustion, is pragmatic. Charge stratification primarily includes stratification of concentration, composition, and temperature, all of which have important influences on ignition, combustion rate, emissions, and load extension. Fuel design and management can be used to optimize SCCI combustion within the full load range and have the potential to control ignition timing and combustion rate, eliminate misfire at light loads and knock problems at heavy loads, and maintain diesel-like thermal efficiency throughout the full engine operational range. Additionally, the HC and CO emissions of SCCI combustion are reduced as compared to HCCI combustion, and NO*x* emissions are dramatically lower than in conventional DI combustion but higher than in HCCI combustion. However, it should be noted that higher stratification will lead to a significant increase in NO*x* emissions.

Fuel design and management based on the combination of port injection and in-cylinder direct injection of fuels with different physico-chemical properties can produce in-cylinder mixture stratification, composition stratification, and temperature stratification. Therefore, the ignition timing, combustion phasing, and heat release characteristics of the full engine operational range can be adjusted for engine performance and emission optimization. Moreover, if supplemented with composition stratification and temperature stratification, iso-octane auto-ignition can be achieved without any additional methods, assisted by an active thermal atmosphere produced from premixed n-heptane.

The opposing physical–chemical properties of diesel fuel and gasoline make them suitable for SCCI combustion using duel-fuel technology or gasoline/diesel blends. For a diesel/gasoline dual-fuel combustion system, NO*x* and soot emissions can be reduced with an increased gasoline (premixed) proportion, yielding an optimal thermal efficiency above 53%. However, increased premixed proportions also result in a rapid increase in pressure-rise rate. For diesel/gasoline-blended fuels, G30 to G50 can cause an 85% reduction in NO*x* emissions, and ultra-low soot emissions can be achieved at full engine load when intake boost is applied.

Future research directions in SCCI combustion: To realize the high efficiency and low emissions in the overall engine operation ranges, the flexible multi-mode combustion processes, such as SI-HCCI-SCCI-SI, DICI-HCCI-SCCI-DICI, or DICI-LTC-SCCIDICI must be necessary to various operating conditions and fuel properties by controlling the $\phi-T$ history. To this target, some basic knowledge should be deeply investigated, including the optimal in-homogenous degree of temperature, composition, and mixture concentration considering different operation cases, closed-loop control strategies of in-cylinder combustion process, the combustion characteristics and emissions during the mode transitions, etc. In the end, the optimization of fuel economy and emissions can be reached to the complete engine operation ranges through an optimum combustion mode transitions. Compared to diesel fuel, due to high octane number and low boiling point, gasoline fuel has potential to extend clean combustion to much higher load. This point has been proved by Kalghatgi et al (PPCI) [389], Splitter et al. (RCCI) [373], Lu et al. (DFSC) [371]. However, research in this area is still limited, and major problems remain to be solved, including combustion stability at low load, pressure oscillations at large load, harmonic combination of fuel stratification, intake pressure and temperature, and EGR. While, the most important problem is to control the high-temperature combustion routes can only occur in the narrow region between soot and NO*x* peninsulas in the $\phi-T$ map, where zero soot and NO*x* emissions are produced.

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Abbreviations

2-EHN: 2-ethylhexyl nitrate
4VVAS: 4-valve variable actuation system
ATAC: active thermo-atmosphere combustion
ATDC: after top dead center
BMEP: brake mean effective pressure
BTDC: before top dead center
CA50: Crank angle at 50% completion of heat release
CAI: controlled auto-Ignition
CFD: computed fluid dynamic
CFR: cooperative fuel research
CN: cetane number
CNG: compressed natural gas
COV: coefficient of variation
DEE: diethyl ether
DICI: direct injection compression-ignition
DME: dimethyl ether
DP-HTHR: dual-phase high-temperature heat release
DFSC: dual-fuel sequential combustion
DMM: dimethyl methane
DTBP: di-tertiary butyl peroxide
EGR: exhaust gas recirculation
FBP: final boiling point
GDI: gasoline direct injection
HCCI: homogenous charge compression-ignition
HRR: heat release rate
HTR: high temperature reaction
HTHR: high temperature heat release
IBP: initial boiling point
ICE: internal combustion engine
IEGR: internal exhaust gad recirculation
IMEP: indicated mean effective pressure
JSR: jet-stirred reactor
LPG: liquefied petroleum gas
LTC: low temperature combustion
LTR: low temperature reaction
LTHR: low temperature heat release
MON: motor octane number
MOP: maximum opening point
MP-HTHR: multiphase HTHR
MRG: methanol-reformed gas
MTBE: methyl tert-butyl ether
NTC: negative temperature coefficient
NVO: negative valve overlap
OI: octane index
OKP: optimized kinetics process
PCCI: premixed charge compression-ignition
PCI: premixed compression-ignition
PFI: port fuel injection
pHCCI: partial HCCI
PLIF: planar laser-induced fluorescence
PRF: primary reference fuel
PRR: pressure rising rate
PPCI: partially premixed compression-ignition
R_p: premixed ratio
qHCCI: quasi-HCCI
RCM: rapid compression machine
REGR: reformed exhaust gas recirculation
RG: reformed gas
RON: research octane number
SAE: Society of Automotive Engineers
SCCI: stratified charge compression-ignition
SI: spark ignition
SOC: start of combustion
SOI: start of injection
TDC: top dead center
TRF: toluene reference fuel
VVL: variable valve lift
VVT: variable valve timing
VCR: variable compression ratio
λ: excess air ratio
η_i: indicated thermal efficiency
ϕ: equivalence ratio