Chapter 3
LTC Fuel Quality Requirements

Abstract In low temperature combustion (LTC) engines, premixed fuel-air mixture is created in the cylinder, and combustion starts by auto-ignition due to compression of the fuel–air mixture during compression stroke. The LTC process involves various physical processes (atomization, evaporation and mixing) and complex chemical reactions occurring in the cylinder. Fuel properties and fuel composition play an important role in all the physical and chemical processes involved in LTC process. Autoignition depends on the evolution of cylinder pressure and temperature with time and autoignition chemistry of the fuel–air mixture. Autoignition chemistry depends on the fuel composition and fuel-air mixture quality (equivalence ratio). This chapter discusses the autoignition characteristics (autoignition chemistry, impact of fuel molecular structure on autoignition, fuel autoignition quality), fuel effects on autoignition and several fuel indices developed for LTC engines. Fuel design and fuel properties/quality required for LTC engines are also discussed in the present chapter.

Keywords Fuel quality • Octane number • Octane index • HCCI number • Fuel design • LTC • RON • Autoignition

3.1 Autoignition Characteristics

In the LTC engine, the fuel and air are premixed (either fully or partially) before the start of combustion. Combustion starts by autoignition at several locations in the combustion chamber due to pressure and temperature rise during compression stroke of engine. The fuel autoignition quality plays an important role in combustion process as the charge is auto-ignited in the cylinder. Different theoretical, empirical and experimental methods exist for describing the autoignition quality of fuels. In theoretical approach autoignition quality is described using chemical kinetics of autoignition process by different types of reaction mechanisms (detailed or reduced mechanism). Empirical models use basic equations derived from experimental data to describe the autoignition quality of fuels in combustion process. In the experimental approach, a test engine or a constant volume chamber is used for comparison of autoignition quality of various fuels. The standard methods for

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quantifying autoignition properties of fuels are RON (research octane number) and MON (motor octane number) for gasoline-like fuels and cetane number (CN) for diesel-like fuels. The autoignition quality of diesel fuel is estimated by CN, which is measured for a given fuel by comparing ignition characteristics with reference fuel in a CFR (corporate fuel research) cetane engine using ASTM D613 test method [1]. The reference fuel is prepared by blending of n-cetane, n-hexadecane (CN = 100) and heptamethyl nonane (CN = 15). The CN of reference fuel having x% volume n-cetane is given by CN = x + 0.15(100 − x). The test fuel is assigned the CN of reference fuel which has the same ignition quality [1]. ASTM methods D2699 and D2700 are typically used to measure RON and MON, respectively, in gasoline-like fuels. RON and MON are estimated on a standardized CFR (corporate fuel research) engine using two sets of operating conditions. During the estimation of RON, CFR engine is operated at 600 rpm speed, inlet temperature of 49 °C and fixed spark timing, while in MON estimation, engine speed is 900 rpm, the inlet temperature is 149 °C and spark timing is adjusted for maximum knock [2]. The mixture of n-heptane and iso-octane is used as reference fuel for octane number measurement. The RON is often higher than MON around 5–10 units for practical hydrocarbons. The difference in RON and MON has led to different definitions of octane number worldwide. For example, only RON is used in the European Union, and in the United States, the average of RON and MON is typically used [2]. The fuel sensitivity (S) is defined as the difference between the RON and MON value (S = RON−MON), which is a measure of the difference in knock tendency for a fuel at different operating conditions [1]. In modern engines, charge condition in the cylinder after compression is different from the RON and especially MON cases. Therefore, suitability of RON and MON needs to be reconsidered. Modern SI engines are “beyond RON” because at a given pressure, the temperature of the unburned mixture is lower than the RON test. Alternatively, the pressure at a given temperature is higher in modern engines than RON test. All the approaches used to improve the SI engine efficiency such as direct fuel injection, higher compression ratio and turbocharging are pushing modern engines further beyond RON [1, 2]. The HCCI engine can be operated well beyond RON and MON. The HCCI engine experiments helped to understand the fuel effects on autoignition with change in operating conditions. The autoignition characteristics of different fuels in LTC engines are discussed in the next subsections.

3.1.1 Autoignition Chemistry

The autoignition process is investigated at a fundamental level by modelling the kinetics of the chemical reactions involved. The ignition process of a commercial transportation hydrocarbon fuel involves hundreds of chemical species participating in thousands of reactions, which makes the whole process very complex. Autoignition occurs when energy released by chain reactions produces exponential increase in temperature of charge in the cylinder. Autoignition starts with initiation

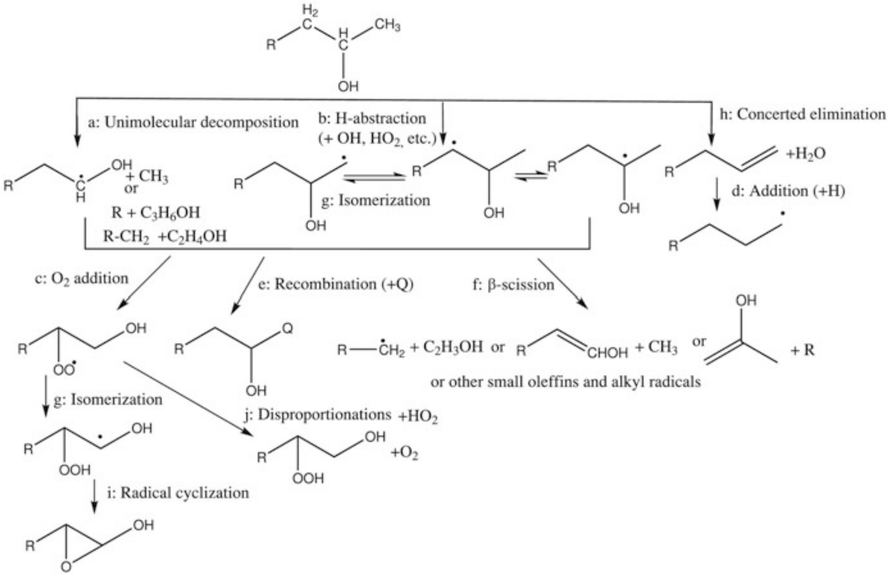


Fig. 3.1 Simplified reaction scheme for hydrocarbon auto-ignition [3]

reactions which generates the radicals from stable species. Chain-branching reactions multiply the number of radicals, which leads to further reaction progress. Chemical reactions involved in the autoignition process can be categorized into ten main types of reactions. Figure 3.1 depicts the summary of simplified reaction scheme of hydrocarbon oxidation by presenting important reactions.

Boot et al. [3] presented the summary of ten main categories of reactions involved in the auto-ignition process as (i) unimolecular decomposition; (ii) hydrogen (H) atom abstraction; (iii) O_2 addition reactions; (iv) other addition reactions of radicals such as H, OH or HO_2, where radicals attach themselves to unsaturated bond sites; (v) recombination reactions; (vi) β-scission; (vii) isomerization; (viii) concerted elimination, two substituents are removed from a molecule in one-step mechanism, forming an unsaturated bond; (ix) radical cyclization; and (x) disproportionation, where two radicals react to produce two different nonradical products. Kinetics of elementary reactions involved in low temperature autoignition process is discussed in detail in the review study [4]. In HCCI combustion engine, the hydrocarbon oxidation process can be divided into low temperature heat release (LTHR), intermediate temperature heat release (ITHR) and high temperature heat release (HTHR) reactions. In Sect. 2.2.2 of Chap. 2, the autoignition reactions involved in HCCI combustion are discussed in detail. Figure 2.4 (Chap. 2) depicts the LTHR, ITHR and HTHR zones as well as single- and two-stage ignition fuels in HCCI engines. Typically fuels containing significant amount of n-paraffins show LTHR characteristics during premixed compression igntion combustion.

Ideally comprehensive chemical models of autoignition process must use all the relevant chemical reactions. However, "comprehensive" schemes cannot be perfectly accurate in the prediction of autoignition process due to uncertainties in the reaction rate constants and their temperature and pressure dependency [1, 5]. Typically detailed reactions mechanisms consist of thousands of reactions. Many practical applications used reduced reaction mechanisms to describe the combustion process [6–8]. Reduced reaction mechanisms are developed by selecting reactions of critical importance for the particular application. Autoignition reaction mechanisms applicable to internal combustion engines are developed for a very few pure compounds. Detailed chemical kinetic models for the oxidation of hydrocarbon fuels are provided in the study [5]. The chemical kinetic schemes are developed for PRFs (primary reference fuels), which contain n-heptane and iso-octane. Conventional gasoline and diesel contain hundreds of species, which have different combustion chemistry than PRFs. Therefore, simplified surrogate fuels are required for representing practical fuels [9]. A surrogate fuel is defined as a fuel composed of a smaller number of pure species, which has the same combustion and emission characteristics as that of targeted practical fuel [1]. The chemical kinetic model of such surrogate fuels is being developed [10–13]. The full chemical kinetic model for surrogate fuels is very large to be used in engine computational models (five-component surrogate has 1328 species and 5825 reactions) [10]. Thus, reduced reaction mechanism is required for autoignition analysis. Empirical autoignition model and experiments can help to understand the autoignition process. Empirical models are discussed in Sect. 3.1.3. Fuel molecular structure also plays an important role in autoignition process, which is discussed in Sect. 3.1.2.

3.1.2 Impact of Fuel Molecular Structure

The chemical composition of commercially available fuel is dependent on the crude oil, refinery processes of oil refineries and season. The HCCI combustion characteristics are very sensitive to the fuel composition, and a fuel standard for advanced combustion is required [14]. Fuel molecular structure affects the auto-ignition characteristics in LTC engines especially in LTHR and ITHR. A typical commercially available gasoline consists of 54.2% total paraffins (10.8% normal paraffins and 43.4% iso-paraffins), 33.6% aromatics, 8.6% olefins, 2.9% naphthenes and 0.88% benzene [1]. A typical diesel contains 44% total paraffins, 29% naphthenes and 25.6% aromatics. Different category of fuel component has different autoignition characteristics. Fuel molecular structure of fuel plays an important role in autoignition characteristics of fuel-air mixture.

The overall autoignition reaction rate is mainly governed by chain-branching reactions (Sect. 2.2.2 of Chap. 2). The chain-branching reaction rate is a function of molecular structure of fuel, pressure and temperature of reactor, equivalence ratio (φ) of mixture and initial concentration of fuel and air [3]. A sufficiently large radical pool is required to autoignite the fuel. At specific initial conditions in the cylinder, the overall autoignition reaction rate is governed by fuel molecular structure. Initial reactions are governed by the type of C-H bond (primary,

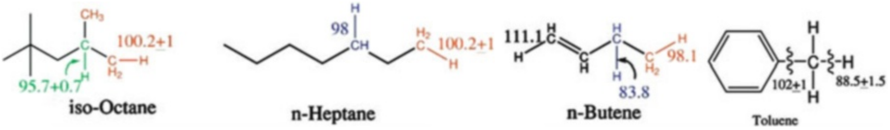


Fig. 3.2 The C–H bond dissociation energy (kcal/mol) for different hydrocarbon fuel component [3, 15]

secondary and tertiary), location of C-H bond in the fuel carbon chain and number of C–H bonds in the fuel molecular structure. Intermediate reactions are governed by hydroperoxyl radical (RO_2) chemistry (propagation and branching reactions). Fuel molecular structure plays an important role in hydroperoxyl radical chemistry in LTHR regime. Terminal reactions are governed by the number and reactivity of intermediate species (termination), which are dependent on fuel structure [3]. The decomposition reactions start with weakest bonds (lowest bond dissociation energy) on the molecular structure of the fuel. Figure 3.2 depicts the C–H bond dissociation energy for different hydrocarbons for different types of C–H bonds (primary, secondary and tertiary bonds). Initiation reactions are followed by H atom abstraction reaction. The bond dissociation energy of C–H bond decreases in the order of primary $>$ secondary $>$ tertiary C–H bond (Fig. 3.2). The molecules having a higher number of primary C–H bonds are more resistant to autoignition reactions. The primary reference fuel n-heptane contains 10 secondary and 6 primary C–H bonds, and iso-octane contains 15 primary, 2 secondary and 1 tertiary C–H bonds. Thus, iso-octane has higher octane number (RON $=$ 100), and it is difficult to autoignite [3].

A study developed an equation to calculate the RON, based on the number of carbon atoms in particular molecular structure by multiple linear regression using data of 58 hydrocarbons [14]. Developed equation for RON calculation is presented in Eq. (3.1):

$$\mathrm{RON}_{\mathrm{calc}} = (-9.13C_2 - 46.0C_d) + (-4.63C_n - 28.0C_{2n}) + 2.30C_b + 107 \quad (3.1)$$

where C_2 is the carbon number of secondary carbon atoms in straight chain, C_d is the dummy variable (if the number of straight chain carbon atoms is higher than 6, $C_d = 1.0$, and if it is less than or equal to 6, $C_d = 0$), C_n is the number of carbon atoms in the naphthene ring, C_{2n} is the number of secondary carbon atoms in the side chains of the naphthene ring and C_b is the number of carbon atoms in the aromatic ring. The calculated RON value correlates well ($R^2 = 0.90$) with experimental data for paraffins, olefins, naphthenes and aromatics. This equation clearly illustrates the importance of molecular structure on the autoignition characteristics. The ignitability of the paraffins increases (RON decreases) with increase in the length of straight chain in the chemical structure (increases rapidly with carbon chain length higher than 6) (see Fig. 3.3 and Eq. 3.1). The ignitability of the hydrocarbon increases with increase in the naphthene ring size and increase in carbon atom number in the side chains of naphthenes, which leads to rapid increase

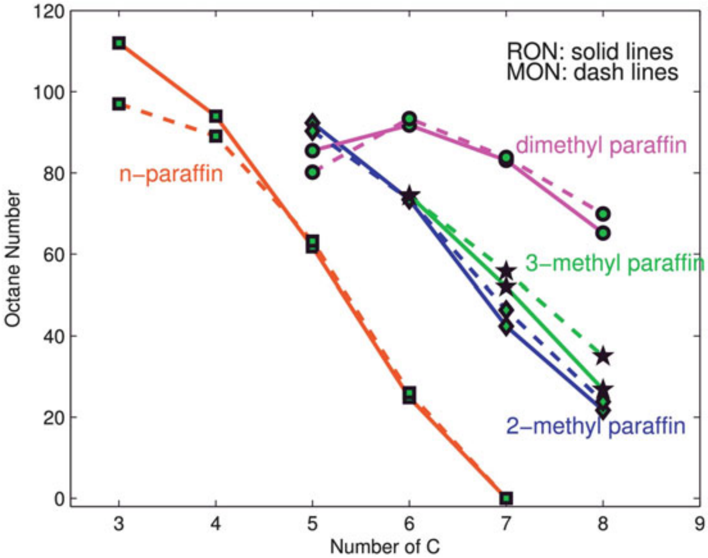


Fig. 3.3 Impact of paraffin chain length and branching on RON and MON [3, 16]

in ignitability or decrease in RON (Eq. 3.1). The ignitability of the hydrocarbon decreases with the addition of aromatics [14].

Figure 3.3 shows that the octane number of fuel decreases with increasing number of carbon atoms in straight chain. This is explained by alkyl radical isomerization reactions at low to intermediate temperatures. The RO_2 radicals (reaction R3, Chap. 2) are very important intermediates in autoignition process. Both alkyl and peroxyl radicals undergo intra-H atom transfer via a transition state ring to produce QOOH, which dominates low temperature chain branching. The isomerization ring strain energy is highly dependent on its size, and larger rings have lower strain energies [3]. The longer average chain length hydrocarbons have more options (more possible site for isomerization reactions) for low energy barrier isomerization reactions and thus higher overall reaction rates in autoignition process leading to higher ignitability or lower octane number (Fig. 3.3). The highly branched paraffins have comparatively lower overall autoignition reaction rates due to drop in average chain length of every branch and higher primary C–H bond (comparatively stronger bond) located at the extremities of molecular structure. This results in lower ignitability and higher RON (Fig. 3.3).

The presence of double bonds and oxygen groups in the fuel affects the possible reaction pathways due to the differences in bond dissociation energies. Additionally, these groups can affect the radical isomerization reactions also. Significant quantity of olefins are present in marketed gasoline. Olefins have a higher RON than paraffins with the same carbon (C) number (Fig. 3.4). The olefinic C bond provides site for addition reactions involving O, H, OH or HO_2 radicals, which initiates the divergence from the paraffinic reaction pathways [3]. The position of

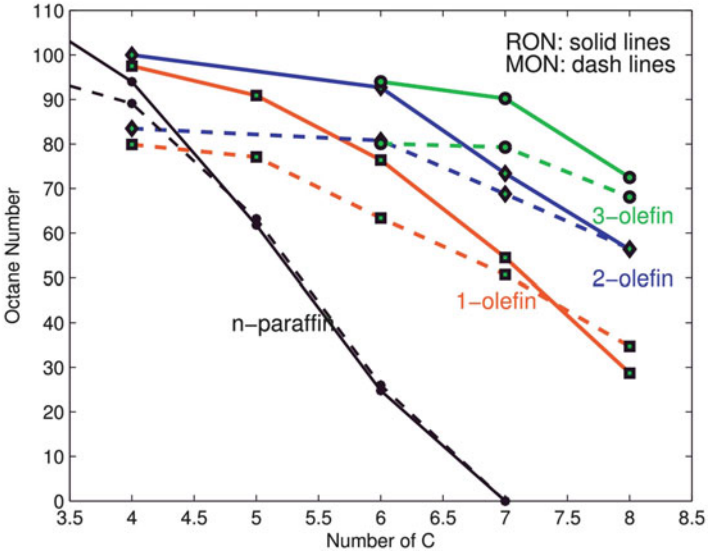


Fig. 3.4 Impact of carbon number and double bond site on olefin reactivity [3, 16]

the double bond in the molecular structure has a significant effect on olefinic autoignition process in the low to intermediate temperature regime [17]. Long-chained olefins having double bond on the extremity tend to show paraffinic-like NTC characteristics [3, 17]. Figure 3.4 also depicts that 3-olefin has higher octane number than 1-olefin.

Almost one-third of gasoline contains aromatics consisting 11.7% toluene, 6.93% m-xylene, 4.04% o-xylene, 3.04% ethyl benzene, 2.58% p-xylene, 1.65% methyl toluene and 1% benzene [1]. Thus, autoignition chemistry of benzene and toluene is important and studied by various researchers [18–22]. Figure 3.5 shows the RON of different aromatic compounds with different number of methyl chains and number of methyl branches. The figure shows that longer side chain aromatics (n-butylbenzene) have lower RON values [14]. The highly stable π-bond in the benzene ring makes H atom abstraction from aromatics difficult. Thus, most aromatics are highly resistant to auto-ignition reactions at low to intermediate temperatures [18]. Benzyl radicals are also resonance stable, and lead to radical–radical reactions in an oxidative environment, which produce even more stable bi-benzyl species. This tendency leads aromatics to both lower propensity for further decomposition and formation of soot during combustion [23]. A more complete discussion on the impact of molecular structure on autoignition characteristics of hydrocarbons can be found in the recent study [3].

Effect of engine operating conditions such as intake air temperature, intake oxygen content and engine speed on ignitability of different hydrocarbon is investigated in HCCI engine [14]. Figure 3.6 shows the effect of intake temperature and engine speed on hydrocarbon ignitability (HI) index of paraffins (n-pentane and

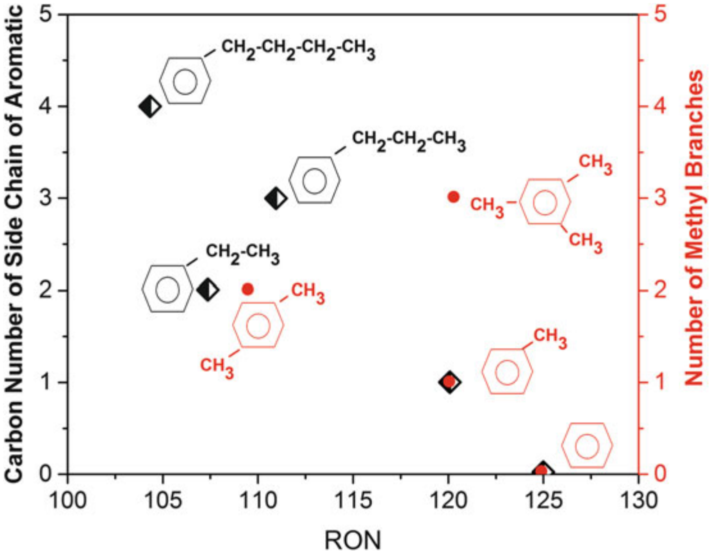


Fig. 3.5 RON versus carbon number of the side chain in aromatics and number of methyl branches in aromatics (Adapted from [14])

iso-octane), naphthenes (cyclohexane and ethyl cyclohexane) and aromatics (toluene, m-xylene and o-xylene) in HCCI engine. The hydrocarbon ignitability index (HI index) is defined as the autoignition characteristic relative to the n-heptane and isooctane scale, based on by octane number measured by the CFR engine [14]. Figure 3.6 shows that the HI indices of the naphthenes increased, and those of the aromatics decreased with the increase in intake air temperature. This observation suggests that the ignitability of the naphthenes decreases and the ignitability of aromatics increases with the increase in intake air temperature. A study suggested that the side chain of naphthenes is responsible for the ignitability improvement, and its effect is stronger at higher intake air temperatures [14]. Oxidation of cyclohexane occurs via two reaction processes (cyclohexane radical reaction and an open-ring reaction process), which are dependent on the charge temperature. The reaction proceeds by cyclohexane radical process at lower low intake air temperature condition, and the LTHR occurs. The naphthene ring opens at the high intake air temperature condition and reactions proceed via open-ring reaction pathway. This reaction pathway does not show LTHR reactions. The two reaction pathways at different temperature lead to different ignitability at higher intake temperature in HCCI engine [14].

In aromatics the chemical ignitability depends on the position of the methyl branch and the side chain length (Fig. 3.5). Ignitability of o-xylene is found higher everywhere in comparison to m-xylene (Fig. 3.6). Differences in the reaction process of o-xylene, m-xylene and p-xylene have been reported in the study [24]. The dehydration reaction in the o-xylene molecule occurs more easily than with m-xylene and p-xylene. This is due to the two methyl groups on fuel molecule

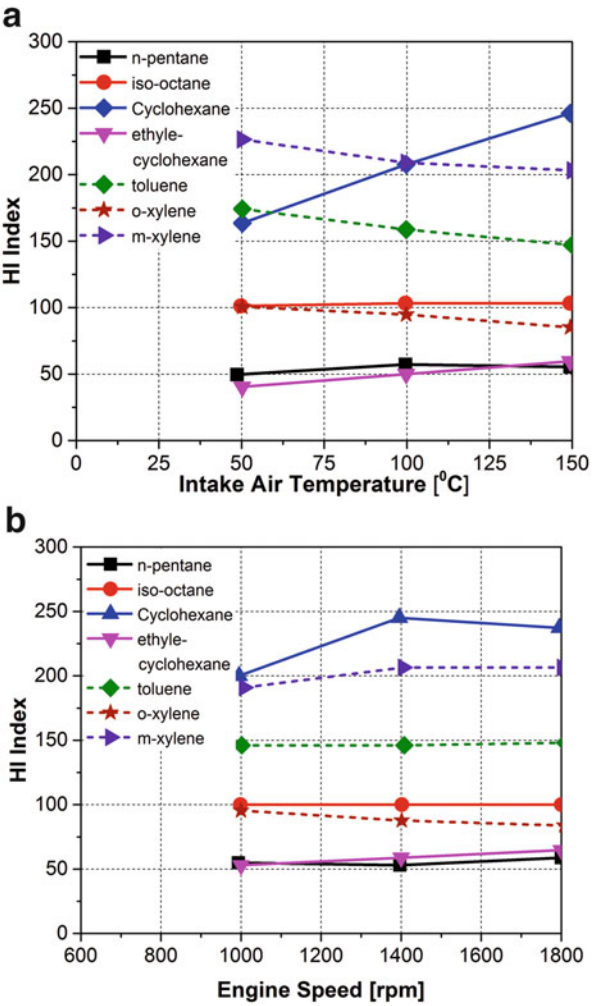


Fig. 3.6 Effect of intake air temperature and engine speed on hydrocarbon ignitability (HI) index in HCCI engine (Adapted from [14])

structure (two methyl groups at the consecutive carbon of the benzene ring) that helps in transition state ring formation during isomerization reaction of o-xylene. This might be a reason of higher ignitability of o-xylene than m-xylene [14].

Figure 3.6b also depicts that the relative ignitability (the HI index) of the naphthenes and aromatics decreases with the increase in engine speed in HCCI engine. With the increase in engine speed, the value of LTHR decreases, and HTHR occurs in the expansion stroke (delayed combustion phasing) particularly for cyclohexane and aromatics with short side chains (toluene, m-xylene, and ethylbenzene) [14]. At higher engine speed, lower time available for LTHR reactions that decreases the amount of LTHR and affects the autoignition characteristics of fuel showing LTHR.

3.1.3 Empirical Auto-ignition Modelling

Empirical approach to describe autoignition is considered as in-between method of theoretical chemical kinetic-based modelling approach and the experimental auto-ignition test methods [25]. The chemical kinetics of HCCI combustion is very similar to the kinetics of knock (end-gas autoignition) in spark ignition engines. Livengood and Wu introduced a method (empirical correlation) to predict the knock conditions for various fuels [26]. This method is also known as knock integral method (KIM) [27]. A study reviewed the five different types of models (based on different complexity and required input data) used to predict the autoignition timings in HCCI engines [28]. Auto-ignition models range from multidimensional CFD models and multizone models to simple control-oriented models. The simplest model uses a threshold temperature to estimate the start of ignition, but it fails to predict combustion phasing at different operating conditions due to dependency of oxidation reaction reactions on species concentration along with charge temperature in the cylinder [29]. The Shell model is also used to predict HCCI ignition timing [30]. Shell model is a lumped chemical kinetic model using only five representative species in the eight generic reactions and only applicable for single-component fuels. Shell model accurately estimates ignition timing over temperature and engine speed sweep, but is less accurate with load variation [28]. A two-step Arrhenius-type reaction rate-based model [31] is used in various studies [32, 33]. In this model the integration of the Arrhenius global reaction rate for the fuel is tracked until it reaches a threshold value defined from experimental data. This model requires instantaneous fuel and oxygen concentrations as well as in-cylinder gas temperature for predicting autoignition, which is impractical for on-board ignition timing control [28]. The KIM is another category of model used for estimating HCCI ignition timing in control-oriented modelling [26]. The KIM is based on an exponential correlation (function of in-cylinder gas pressure and temperature) to predict the auto-ignition characteristics of a homogeneous fuel–air mixture [34].

The KIM is a common empirical method used in the estimation of HCCI ignition timings. The basis of the correlation stems from the ignition delay of various fuels using a rapid compression testing machine [26]. The resulting empirical relationship in the general form is provided in Eq. (3.2):

$$\tau = Ae^{\left({}^{b}/_{T}\right)p^{n}} \tag{3.2}$$

where τ is the ignition delay (or induction time), p is the charge pressure as a function of time, T is the charge temperature as a function of time and A, b and n are empirical constants. Ignition delay or induction time is defined as the time between the end of compression and autoignition (marked by heat release) in rapid compression machine [1]. The relatively more reactive mixture has lower ignition delay (τ).

Livengood and Wu proposed the functional relation between the concentration ratio, $(x)/(x)_c$, of the significant species in the autoignition reaction and the relative time, t/τ. The $(x)_c$ is the critical concentration ratio, which is the concentration of the species at the end of the reaction. The ignition correlation of Livengood and Wu in terms of the crank angle instead of time (as typical engine combustion characteristics measured on crank angle basis) is shown in Eq. (3.3) [28]:

$$\frac{x}{x_c} = \int_{\theta_0=0}^{\theta=\theta_e} \frac{1}{\omega\tau} d\theta = \int_{\theta_0=0}^{\theta=\theta_e} \frac{1}{A\omega e^{\left(b/T\right) p^n d\theta = 1.0}} \tag{3.3}$$

where θ_e is the crank position at which autoignition or knock occurs and θ_0 is the initial crank position where integration starts. The engine speed (ω) is signified in revolutions per minute (rpm), the pressure in kPa and the temperature in K.

In this model, instantaneous pressure and temperature of cylinder charge are required to estimate the ignition timings. The measurement of in-cylinder pressure on engine is difficult and expensive which limits the utilization of this model for real-time control. A study [28, 35] presented modified knock integral model (MKIM) for estimation of HCCI ignition timings using intake valve closing (IVC) pressure and temperature, equivalence ratio and instantaneous volume. The MKIM is presented by Eq. (3.4):

$$\int_{\theta_{\mathrm{ivc}}}^{\theta_{\mathrm{soc}}} \frac{\phi^B}{A\omega \exp\left(\frac{C\left(P_{\mathrm{ivc}} v_c^{k_c}\right)^D}{T_{\mathrm{ivc}} v_c^{k_c-1}}\right)} d\theta = 1.0 \tag{3.4}$$

where θ is the engine crank angle and B, C and D are constant parameters. k_c represents the average polytropic coefficient. The value of the expression being integrated increases as the point of SOC is approached. A and v_c are determined by

$$v_c(\theta) = \frac{V_{\mathrm{ivc}}}{V(\theta)}, A = E_1 \mathrm{EGR} + E_2 \tag{3.5}$$

where E_1 and E_2 are constant parameters and the cylinder volume, $V(\theta)$, is calculated at any crank angle using slider crank mechanism.

A study investigated the validity of correlation proposed by Livengood and Wu in HCCI engines for various fuels with practical interest (hydrogen, methane, ethanol and n-heptane) [36]. The study concluded that the method predicts ignition timings quite accurately for the fuels (hydrogen, methane and ethanol) with single-stage heat release (no LTHR). However, KIM underpredicts the ignition time when ignition takes place after the TDC for all three cases because KIM cannot account for slowing down the oxidation chemistry due to cooling effect of the expansion. The study also showed that the KIM method fails to accurately predict the ignition timing for two-stage heat release (LTHR and HTHR) fuel (n-heptane), and it overpredicts the ignition timing. Another study describes the ignition delay as a combination of a low temperature regime and high temperature regime induction time, and each stage is described by an Arrhenius equation [37]. The study showed that this is a convenient and flexible method for describing the ignition delay of a wide range of fuels including linear paraffins, iso-paraffins, olefins, aromatics and alcohols.

3.1.4 Fuel Effects on Autoignition in LTC Engines

Gasoline and diesel fuel contain hundreds of components and each component has its specific autoignition temperature. The variations in the temperature and fuel composition make autoignition control very difficult in HCCI combustion. Understanding of fuel effects on autoignition process is required to describe and predict the autoignition process in HCCI combustion. Autoignition temperature and LTHR are closely coupled with fuel autoignition qualities in HCCI engines. Gasoline-like fuels with an octane number lower than 83 show LTHR in HCCI combustion [38]. Diesel-like fuels or high cetane number fuels typically exhibit LTHR in HCCI combustion, and LTHR disappears for fuels having cetane number less than 34 (CN $<$ 34) [39]. Fuel structure is strongly related to LTHR (Sect. 3.1.2), and small variation in chemical composition can change the HCCI combustion characteristics [40].

Figure 3.7 illustrates the effect of PRF fuel composition on LTHR rate in HCCI combustion. The LTHR decreases with increase in PRF octane number (increase in

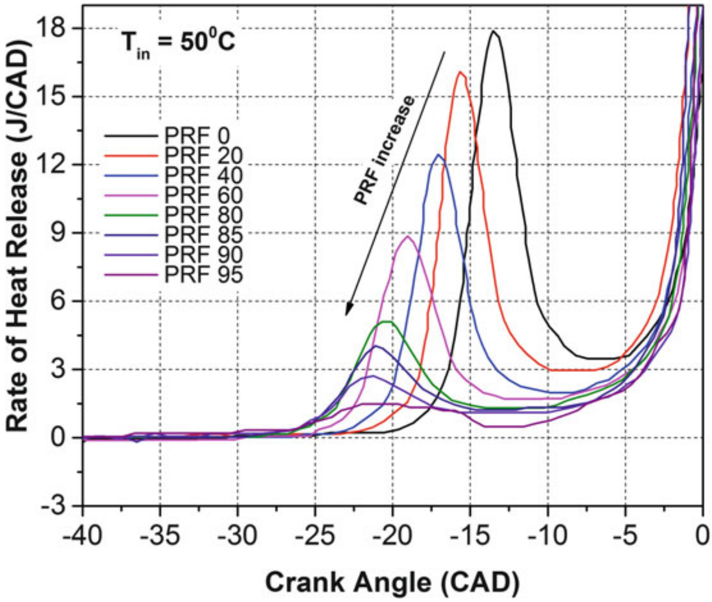


Fig. 3.7 Effect of PRF fuel composition (different n-heptane concentration) on LTHR in HCCI combustion (Adapted from [41])

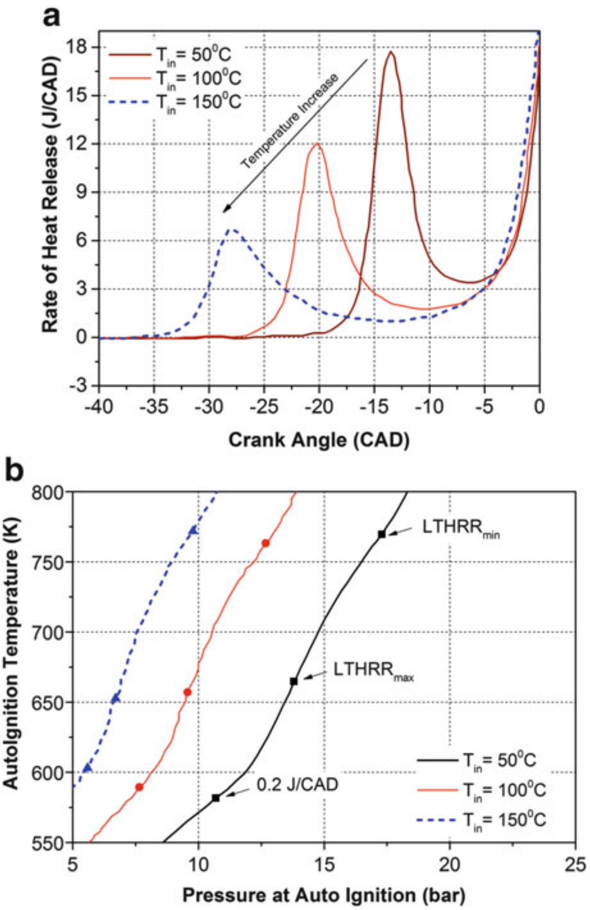


Fig. 3.8 Effect of intake temperature on (**a**) LTHR and (**b**) autoignition temperature for PRF0 (n-heptane) in HCCI combustion (Adapted from [41])

iso-octane content). The LTHR depends on concentration of straight chain paraffins (Sect. 3.1.2), and therefore as n-heptane concentration in fuel decreases (increase in PRF octane number), the amount of LTHR decreases.

Figure 3.8 shows the effect of intake temperature on LTHR and autoignition temperature in HCCI engine using PRF0 (pure n-heptane). The LTHR is higher at lower intake air temperature and decreases with increase in inlet temperature. The main reaction containing alkyl–peroxyl radical formation (reaction R3; Chap. 2) is a reversible reaction and responsible for LTHR. This reaction is highly dependent on temperature and an increase in temperature shifts the reaction towards the reactant side. Therefore, increasing inlet temperature leads to lower amount of LTHR (Fig. 3.8). At lower inlet temperatures, higher compression ratio is used to achieve a constant combustion phasing, and higher pressure is known to increase the LTHR [41]. For higher octane PRF, LTHR diminishes at higher intake temperatures, which leads to delayed start of combustion. Figure 3.8b also depicts that the maximum value of low temperature heat release rate ($\mathrm{LTHRR}_{\mathrm{max}}$) occurs at almost

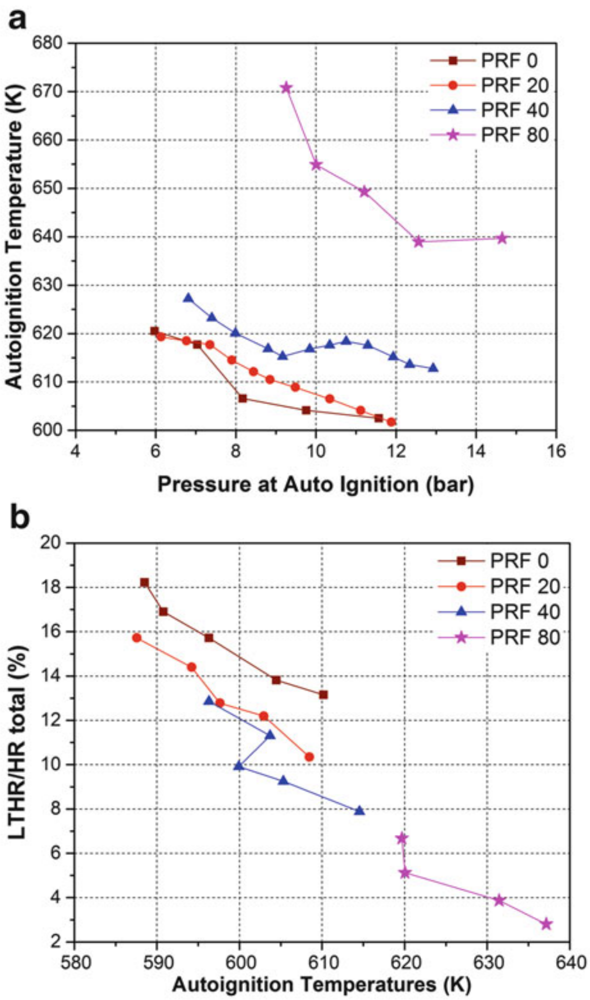


Fig. 3.9 Effect of PRF fuel composition on (**a**) autoignition temperature, and (**b**) LTHR in HCCI engine (Adapted from [41])

same temperature for each test condition. In this figure, autoignition (start of LTHR) is defined as the point where heat release rate of 0.2 J/CAD has reached. The LTHR starts decreasing after reaching $\mathrm{LTHRR}_{\max}$ in each operating conditions. At lower intake temperature, autoignition temperature is also lower (Fig. 3.8b).

Figure 3.9 shows the effect of PRF composition on autoignition temperature and LTHR fraction. The LTHR fraction is shown in the figure as percentage of total heat release in the cylinder. Different points for each test fuel in Fig. 3.9 correspond to the different inlet air temperatures. Autoignition temperature increases with increase in octane number of the fuel. Fuels having extensive LTHR show similar autoignition characteristics, and autoignition starts at almost the same temperature regardless of the cylinder pressure. The n-heptane (PRF0) auto ignites around

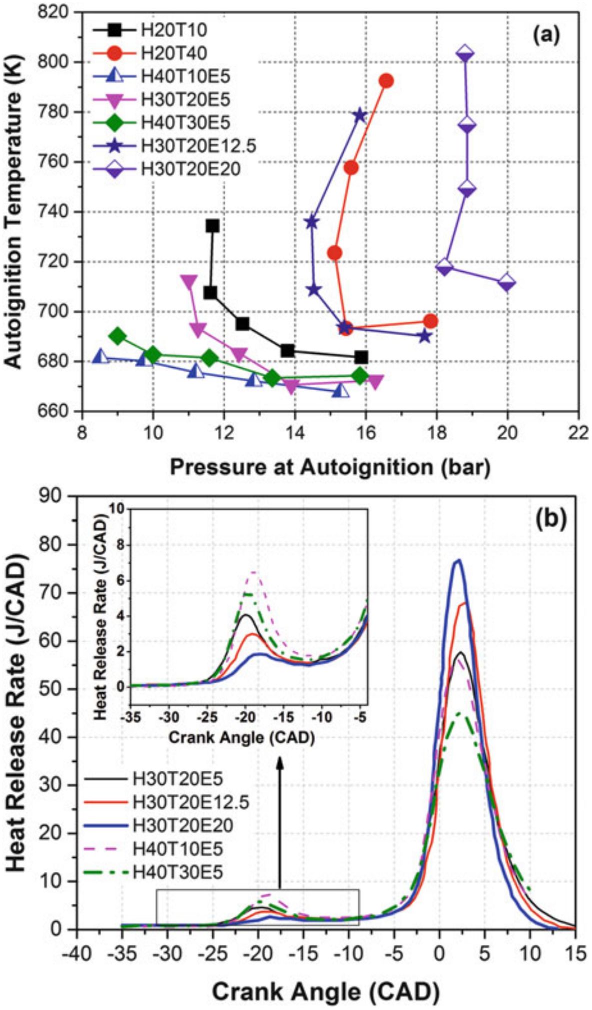


Fig. 3.10 Effect of TERF fuel composition on (**a**) autoignition temperature, and (**b**) LTHR in HCCI combustion (Adapted from [42, 43])

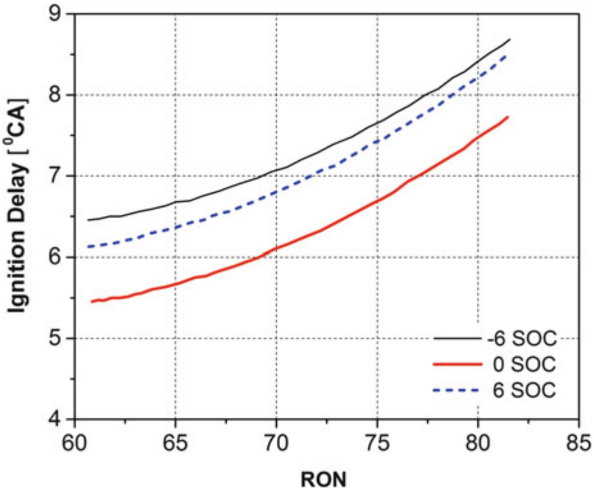
570 K, with a weak trend that comparatively higher autoignition temperature is required for lower cylinder pressure. With decrease in LTHR, autoignition temperature rises quickly [41]. Figure 3.9b depicts almost linear correlation between the amount of LTHR and autoignition temperature. All the test operating conditions having detectable LTHR (>1% and with a LTHR_{max}) ignited at temperatures below 650 K (Fig. 3.9b).

Figure 3.10 illustrates the effect of toluene and ethanol content on autoignition temperature and LTHR in HCCI combustion. Five data points on the curve (Fig. 3.10a) represent the five intake temperature for a particular fuel. Fuels designated as HxTyEz contains x% of n-heptane, y% of toluene, z% of ethanol and (100-x-y-z) % of iso-octane. Ethanol and toluene are known to reduce LTHR reactions by consuming radicals during LTHR regime [44, 45]. Generally, autoignition temperature increases with increase in intake temperature for all the test fuels, but the level of change in autoignition temperature is different for different fuels (Fig. 3.10a). The curve for toluene ethanol reference fuels (TERF) is similar to PRFs (Fig. 3.9a). Toluene addition in the fuel increases the auto-ignition temperature (see case H20T10 and H20T40), which can be seen as upward shift in the graphs as toluene content increases. An increase in autoignition temperature is observed mainly at higher intake temperatures due to the lower LTHR. Autoignition temperature differs slightly at lowest intake temperatures. Fuels depicting LTHR at all five intake temperatures, autoignition occurs at similar charge temperatures. Fuels with little or no LTHR have comparatively larger difference in autoignition temperatures. Radical quenching effect of ethanol can be seen by comparing the amount of LTHR for three fuels with a constant amount of n-heptane (30 vol.%) and toluene (20 vol.%) but varying amounts of ethanol (5, 12.5, 20 vol.%) (Fig. 3.10b). Toluene quenching effect is also depicted in Fig. 3.10b by comparing two fuels having constant amount of n-heptane (40 vol.%) and ethanol (5 vol.%) but varying amounts of toluene (10, 30 vol.%). The lower LTHR for the particular fuel with a higher concentration of ethanol or toluene shows the quenching effect. The figure shows that toluene has the weaker LTHR quenching effect than ethanol, despite the higher RON of toluene than ethanol (120 compared to 109) [43].

Gasoline partially premixed combustion (PPC) is another LTC strategy that demonstrated higher operating range and better combustion control, while keeping the benefits of HCCI combustion (Sect. 2.5.2 of Chap. 2). In PPC mode, ignition delay and LTHR have an important role in ignition characteristics. Premixed combustion phase in PPC needs mixing of fuel and air before ignition starts. The desired premixing is achieved by longer ignition delay. During ignition delay period, physical processes (droplet evaporation, mixing of fuel with air and heating due to compression) and chemical process (formation of radicals and intermediates) occur in the engine cylinder [27]. Effect of fuel properties on PPC relates through charge cooling effect during evaporation, mixing process and fuel ignitability (reactivity) [46]. At constant combustion phasing, ignition delay is correlated with fuel RON (Fig. 3.11). Figure 3.11 shows that the ignition delay increases with an increase in RON value for different start of combustion (SOC) operation in PPC mode because fuel reactivity decreases with increase in RON. The ignition delay is found to decrease with retarding SOC, and minimum around SOC at TDC position (0 CAD). Until SOC reaches TDC position, ignition delay decreases due to higher pressure and temperature of air during compression. Air pressure and temperature decrease for SOC after TDC, which also leads to higher ignition delay.

Duration of LTHR reaction depends on the ignition delay. Prolonged ignition delay gave an increased duration of LTHR in PPC engine. Figure 3.12 shows the variations of ignition delay, LTHR duration and LTHR fraction with engine load at constant combustion phasing of 6 CAD after TDC and 1500 rpm. Low load limit achieved with stable combustion for low and high octane fuels is also indicated in Fig. 3.12. The low load limit is defined as the point where ambient intake

Fig. 3.11 Predicted ignition delay as a function of RON in PPC engine at 8 bar IMEP and 1500 rpm (Adapted from [47])



temperature is not enough for stable combustion. The lowest stable load achieved with higher octane number fuel is higher in comparison to lower octane number in PPC. Justification of trend can be found in Sect. 2.5 of Chap. 2. Ignition delay period decreases with increase in engine load for all fuels above the low load limits due to the low temperature at start of injection (SOI). The SOI timings are adjusted to achieve the constant combustion phasing for all the test conditions. Fuel is injected at lower cylinder pressure-temperature at early (advanced) SOI timings. Ignition delay decreased again when λ increases (lower IMEP), in case of below the low load limit conditions. Apparently, the higher oxygen fraction has a stronger impact on the ignition delay than the decrease in charge temperature [48]. LTHR reaction rate depends on both fuel composition and gas temperature in the combustion chamber. Above the low load limit, duration of LTHR decreases with an increase in engine load. Fraction of LTHR is a function of engine load (Fig. 3.12b), and LTR fraction increased with decrease in engine load because of reduction in cylinder temperature. The fraction of the LTHR decreased with increased load from about 5% at 2 bar IMEP to about 3% at 8 bar IMEP [48].

Figure 3.13 shows the effect of inlet oxygen content and fuel composition on ignition delay and LTHR fraction (also referred as low temperature reaction (LTR) fraction in few studies) in PPC combustion. Ignition delay depends on the injection parameters (injection quantity, injection timing and injection pressure) and engine operating parameters (air charge conditions, load, engine speed, combustion chamber geometry and swirl rate) for a particular fuel. Figure 3.13a shows the variations of ignition delay at constant engine speed and load conditions for constant combustion phasing, where fuel injection timing and duration are adjusted to achieve the load (IMEP 8 bar) and combustion phasing (3 CAD aTDC). Experiment is conducted at absolute inlet pressure of 2.8 bar. Ignition delay is longer for higher RON fuel due to high resistance to autoignition, and distinct difference in ignition delay is observed proportional to difference in RON for each fuel. At

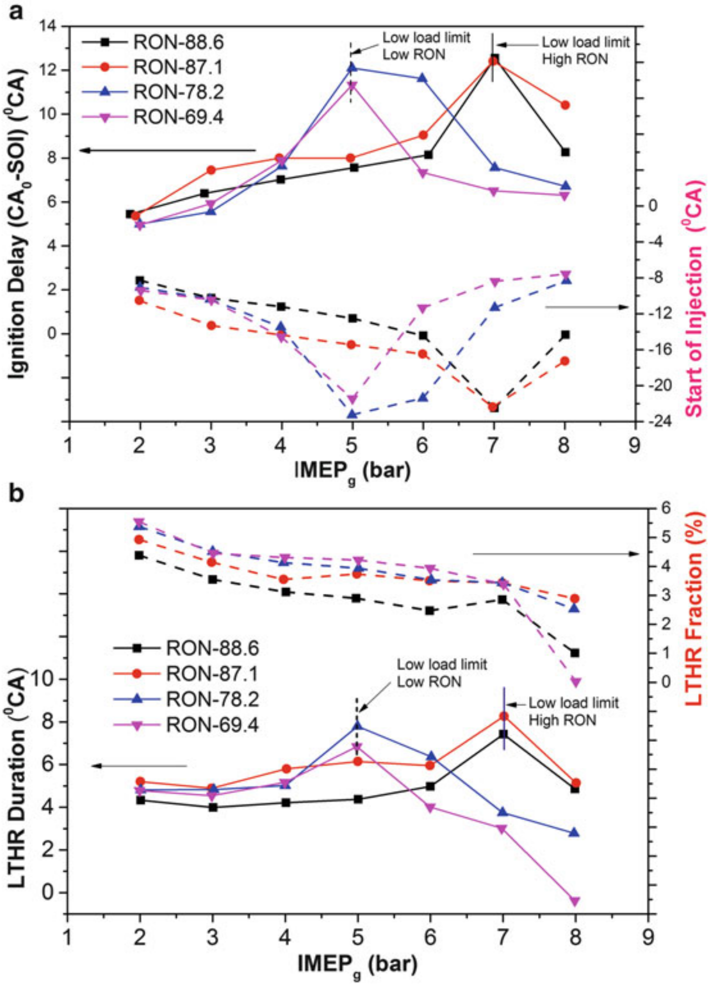


Fig. 3.12 Variation of ignition delay, LTHR duration and LTHR fraction with engine load in PPC at constant combustion phasing of 6 CAD after TDC (Adapted from [48])

lower oxygen concentration, more ambient gas needs to mix with fuel for release of same energy. Therefore, additional time is required for the mixing and hence ignition delay is higher.

In HCCI combustion, LTHR increases with increase in n-heptane content and decreases with increase in iso-octane content [49, 50]. In PPC combustion, LTHR increases with decrease in n-heptane content and increase in EGR rate. This trend is opposite to the trend observed in HCCI combustion. The SOI is advanced to achieve constant combustion phasing for high RON fuels, and advancing SOI increases LTHR phase due to lower cylinder temperature and pressure. The inlet oxygen concentration has stronger impact on LTHR than fuel composition for PRF fuel (Fig. 3.13a) [47].

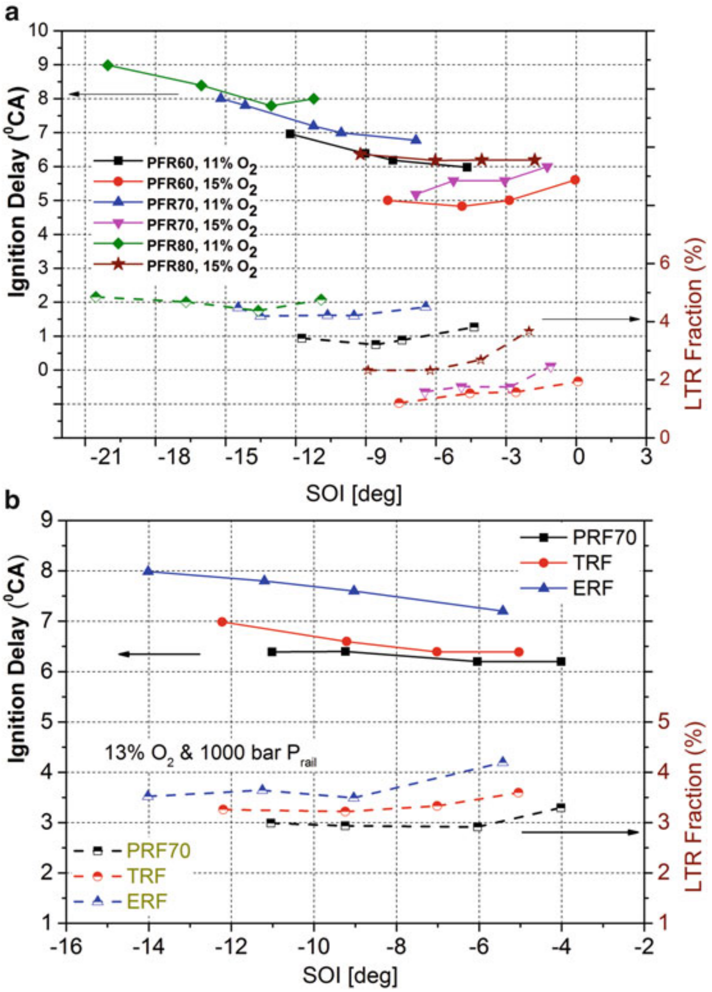


Fig. 3.13 Ignition delay and LTHR as a function of SOI for different (**a**) PRFs and oxygen content, (**b**) ERF and TRF (Adapted from [47])

Figure 3.13b depicts the effect of fuel composition (especially fuel containing aromatic and alcohol) on ignition delays and LTHR phase in PPC. A base fuel PRF70 is compared to TRF (toluene reference fuel) and ERF (ethanol reference fuel). The n-heptane concentration is the same for all the fuel (30% by volume) fractions, and iso-octane in PRF70 is replaced by 15% toluene for TRF fuel and by 10% for ERF fuel. To maintain the same combustion phasing, SOI is advanced for TRF by one degree. Ignition delay is higher for TRF and ERF fuel in comparison to PRF70 as octane number is higher for these fuels. Ignition delay is more influenced by ethanol than toluene. Ethanol and toluene have amplified the LTHR regime in PPC mode which is the opposite of HCCI mode trend (Fig. 3.13b) [47]. However, ethanol has higher impact on LTHR than toluene in PPC combustion.

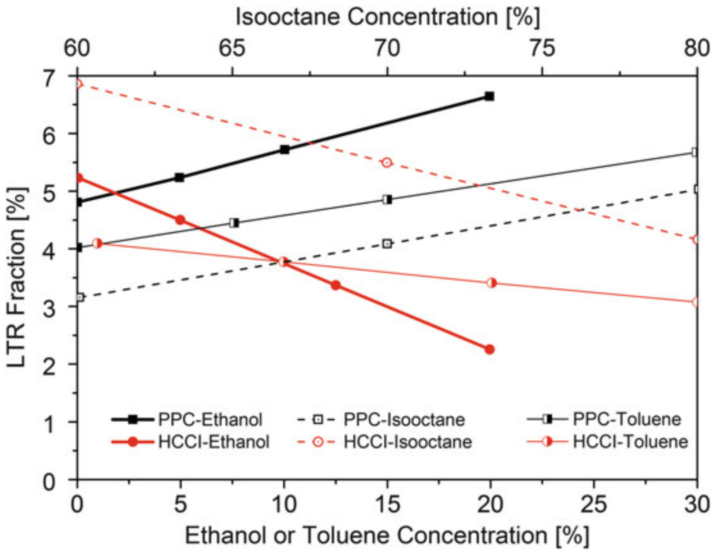


Fig. 3.14 LTHR fraction as a function of ethanol, toluene and iso-octane concentration in HCCI and PPC combustion (Adapted from [51])

Figure 3.14 compared the LTHR (or LTR) fraction in HCCI and PPC combustion at various fuel compositions (different ethanol, toluene and iso-octane concentrations in fuel) at constant engine load. The figure shows that LTHR fraction increases with increase in ethanol concentration with a slope of 0.08 in PPC combustion. However, LTHR fraction decreases with a slope of −0.1 with increase in ethanol content in HCCI combustion mode. Similarly, LTHR fraction increases with increase in toluene in PPC and decreases in HCCI combustion mode. For both PPC and HCCI combustion, the steepness of the slopes is similar but in reverse direction. Figure 3.14 also depicts that ethanol has a higher effect on LTHR fraction than toluene. Similar trend is also observed for iso-octane fraction.

In summary, fuel effect on LTHR in PPC is reversed as compared to HCCI mode. It is suggested that chemical fuel effects dominate over physical effects for port-injected HCCI. However, the processes involved in LTHR regime are more complex in PPC mode than in HCCI mode. The strong relation between LTHR and ignition delay in PPC mode shows that the ignition quality plays a key role in LTHR regime [51].

3.1.5 Autoignition Quality Test Limitations

The cetane number (CN) and octane number (ON) are the main parameters used to characterize chemical properties of fuel in conventional CI and SI engines, respectively. The HCCI operating conditions cover both the ignition quality (CN) and anti-knock quality (ON) at both lean (low load) and rich (high load) limit conditions. Thus, conventional CN or ON may not be optimal parameter for fuel characterization in HCCI engines. Studies suggested that HCCI ignition characteristics cannot be estimated by conventional measurement of autoignition quality of fuels (RON, MON or CN) [52].

The compression ratio required for auto-ignition of different kinds of paraffin does not rank with ON [53]. Issues related to RON and MON for characterizing the auto-ignition behaviour in HCCI engine are further investigated [43, 54–56]. These studies concluded that RON and MON methods do not describe pressure fluctuations from auto-ignition in the end gas, but it rather describes the rate of change of pressure prior to knocking. Additionally, the pressure at a given temperature is higher in modern engines than RON test.

No correlation is found between combustion phasing (CA_{50}) and RON or MON in HCCI combustion with negative valve overlap by testing 15 different fuels with high octane numbers [57]. Another study showed that fuel composition affects the ignition delay for fuels with same RON or MON, and thus neither RON nor MON is a complete predicator of autoignition quality in HCCI engines [58]. Therefore a new index is required for estimating fuel performance in HCCI combustion engines.

3.2 LTC Fuel Index

In HCCI engine, fuel composition strongly affects the combustion phasing and magnitude of heat release rate (HRR). Fuel with high olefin/aromatic content can reduce the maximum HRR and cylinder pressure as much as 20% and shift the maximum HRR position up to 10 CAD in HCCI engine operated at similar RON and MON fuels with different composition [58]. A study showed that the marketed gasoline has variations in aromatic content ranges from 4% to 54% and olefinic fraction ranges from 0% to 30% [59]. Fuel composition variability makes HCCI engine control more challenging. Fuel composition effect on combustion characteristics and variations in fuel composition in pump fuels leads to the development of newer methodology for prediction autoignition characteristics in LTC engine. Next subsections present the several fuel index developed to describe the autoignition characteristics of LTC engine fuel.

3.2.1 Octane Index

To describe the autoignition characteristics of HCCI combustion, Kalghatgi et al. developed a parameter called octane index (OI), which better correlates the combustion phasing [1, 60]. The octane index is defined by Eq. (3.6):

$$\mathrm{OI} = (1 - K).\mathrm{RON} + K.\mathrm{MON} = \mathrm{RON} - K.S \tag{3.6}$$

The value of parameter K depends on engine operating conditions (value can be positive, zero or negative), and S is fuel sensitivity (S=RON−MON). Fuel sensitivity depicts the response of a particular fuel at higher intake temperatures for knock tendency relative to iso-octane and n-heptane [61]. Fuel sensitivity is zero for PRFs and, hence, OI for PRF is equal to RON. The value of K is 0 and 1 for RON and MON test conditions, respectively. The higher OI of fuel means more resistant to autoignition and leads to retarded combustion phasing in HCCI engine.

The OI represents the combustion characteristics of the fuel. Combustion phasing (CA_{50}) is proposed to be a linear function of RON and MON. The K value is estimated by regression analysis [1]:

$$\mathrm{CA50} = a\mathrm{RON} + b\mathrm{MON} + c \tag{3.7}$$

$$\mathrm{CA50} = c + (a + b)\mathrm{OI} \tag{3.8}$$

where $\mathrm{OI} = ((a/(a+b))/\mathrm{RON} + ((b/(a+b))/\mathrm{MON})$ and K is defined as $b/(a+b)$.

The K value strongly depends on the temperature at 15 bar cylinder pressure (T_{comp15}) and increases with T_{comp15} [62]. T_{comp15} is a function of physical state in the cylinder (based on engine speed, intake temperature, etc.), and K is dependent on engine operating condition, but not on the fuel properties. A predictive equation for K as a function of T_{comp15} and the relative air/fuel ratio (λ) is obtained and presented in Eq. (3.9):

$$K = 0.00497^{*}T_{\mathrm{comp15}} - 0.15^{*}\lambda - 3.67 \tag{3.9}$$

At every engine operating condition, there exists an ideal fuel with $\mathrm{OI} = \mathrm{OI}_0$ where combustion phasing (CA_{50}) is at TDC. OI_0 increases with increase of compression pressure and temperature at TDC position. OI_0 value reduces with increasing λ and engine speed. OI_0 can be recognized as engine's fuel requirement.

The OI is a good indicator of autoignition characteristics for most of the PRF blends and surrogates composed of a few pure chemical components. However, OI does not correlate well for gasoline fuels containing ethanol, naphthenes and aromatics [61, 63, 64]. These species are typically found in commercial gasoline worldwide.

A recent study improved the OI and proposed a new OI model (JKZ model) [61]. The modified OI is shown in Eq. (3.10):

$$\begin{aligned}\mathrm{OI}_{\mathrm{modified}} = {} & \mathrm{RON} - \mathrm{K}'.\mathrm{S} + \kappa(\mathrm{Aromatics})^2(\mathrm{Olefines} + \mathrm{Saturates}) \\ & + \varepsilon(\mathrm{Aromatics.Ethanol})\end{aligned} \tag{3.10}$$

The two new parameters (κ and ε) are used in conjunction with K′ defined previously in order to keep the same convention as Kalghatgi's OI. In this model, combustion phasing (CA_{50}) is related to RON and MON value of fuel by Eq. (3.11):

$$\mathrm{CA}_{50} = c' + a'\mathrm{RON} + b'\mathrm{MON} + d\,(\mathrm{Aromatics})^2\,(\mathrm{Olefins} + \mathrm{Saturates}) + e(\mathrm{Aromatics.Ethanol}) \tag{3.11}$$

In Eq. (3.11), aromatics, olefins, saturates and ethanol represent the volume fraction of each respective component in the fuel. The parameters K′, κ and ε are calculated as

$$k = b'/(a' + b'); \kappa = d/(a' + b'); \varepsilon = e/(a' + b');$$

Modified OI is more capable of capturing the auto-ignition characteristics of the refinery stream fuels for all the intake temperature conditions, especially low intake temperatures.

3.2.2 CAI/HCCI Index

Shibata and Urushihara [65] developed a HCCI index based on MON and amounts of five components (n-paraffin (nP), iso-paraffin (iP), olefin (O), aromatics (A) and oxygenates (OX)). The Shibata–Urushihara HCCI index is given in Eq. (3.12):

$$\text{S-U HCCI Index (abs)} = m.\mathrm{MON} + a.(\mathrm{nP}) + b.(\mathrm{iP}) + c.(\mathrm{O}) + d.(\mathrm{A}) + e.(\mathrm{OX}) + Y \tag{3.12}$$

All fuel component concentration in Eq. (3.12) is the percent by volume, and *m*, *a*, *b*, *c*, *d*, *e* and *Y* are temperature-dependent constants. The value of coefficient "*e*" depends upon the specific oxygenate in the fuel formulation (ethanol, MTBE or ETBE). The SU–HCCI index corresponds to the crank angle timing for 20% completion of the HTHR.

The same study also developed HCCI index in terms of RON, which is more widely used index, and HCCI index expression is presented in Eq. (3.13) with a separate set of coefficients [65]:

$$\text{S-U HCCI Index (abs)} = r.\mathrm{RON} + a'.(\text{n-p}) + b'.(\text{i-p}) + c'.(\mathrm{O}) + d'.(\mathrm{A}) + e'.(\mathrm{OX}) + Y' \tag{3.13}$$

Studies with different gasoline composition suggest that SU–HCCI index poorly predicts the autoignition characteristics of HCCI combustion [64, 66].

Another group proposed a HCCI index based on the fuel's tendency to decrease or increase the HCCI operating region [67]. This index compares the operating area (in HCCI mode) achieved with the given fuel to the HCCI operating area achieved with the reference fuel. Figure 3.15 illustrates the definition of HCCI index. Moreover, a good HCCI fuel must not deteriorate the full load performance. A modified HCCI index is proposed and presented by Eqs. (3.15) and (3.16) to have

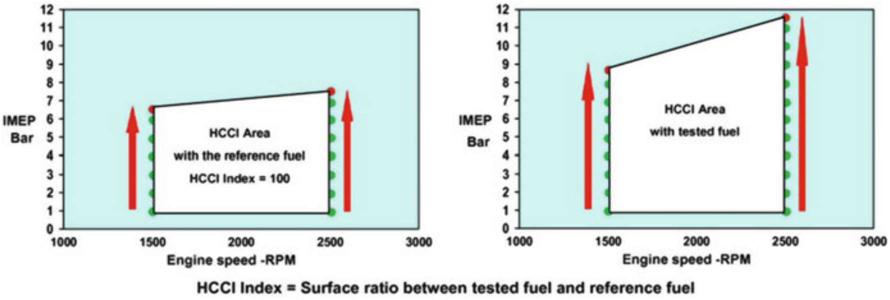


Fig. 3.15 HCCI index definition [67]

higher importance to full load operation in conventional mode, which eliminates the improvement allowed in HCCI mode:

$$\text{HCCI index} = \frac{\text{Tested Fuel HCCI Surface}}{\text{Ref.Fuel HCCI Surface}} \tag{3.14}$$

$$\text{Mod.HCCI index}(1) = 0.8 \times \frac{\text{Tested Fuel HCCI Surface}}{\text{Ref.Fuel HCCI Surface}} \times 100 + 0.2 \times \frac{\text{Max Power Tested Fuel}}{\text{Max Power Ref.Fuel}} \times 100 \tag{3.15}$$

$$\text{Mod.HCCI index}(2) = \frac{\text{Tested Fuel HCCI Surface}}{\text{Ref.Fuel HCCI Surface}} \times \frac{\text{Max Power Tested Fuel}}{\text{Max Power Ref.Fuel}} \times 100 \tag{3.16}$$

A similar procedure is also used to evaluate the fuel effect on the controlled autoignition (CAI) combustion [68, 69]. The CAI index is used to precisely quantify the effect of fuel on four CAI zones defined as low-speed/low load, low-speed/high load, high-speed/high load, and high-speed/low load zones. The HCCI index is used to compare HCCI operating region achieved from the tested fuel with that achieved from the reference fuel.

3.2.3 *Lund–Chevron HCCI Number*

Lund–Chevron HCCI number is developed to fulfill the need of a HCCI number analogous to that of RON and MON for SI engines. To estimate HCCI number, first a set of reference curves of the compression ratio (CR) is generated for combustion phasing (CA_{50}) at 3° aTDC using PRFs at five different intake temperatures (50–150 °C) [66]. A quadratic function of CR with octane number is obtained by fitting quadratic relation in PRF data (PRF60–100) as shown in Eq. (3.17):

$$\mathrm{CR} = a.x^2 + b.x + c \tag{3.17}$$

where “x” is the volume % of iso-octane in the primary reference fuels used to develop the correlation. The constants a, b and c obtained by curve fitting and their values are different for different intake temperatures. For particular fuel and engine operating conditions of interest, the autoignition CR is plotted vs. RON, along with the reference quadratic curve for the PRFs at the same conditions. The HCCI number of fuel is assigned equal to the RON of the PRF that had the same CR. The quadratic equation can be rewritten for calculating HCCI number from CR by Eq. (3.18) [43]:

$$\text{HCCI number} = -\frac{b}{2.a} + \sqrt{\left(\frac{b}{2.a}\right)^2 - \left(\frac{c - \mathrm{CR}}{a}\right)} \tag{3.18}$$

In this manner, HCCI numbers can be determined for each test fuel at engine operating condition of interest. The Lund–Chevron HCCI number is found to be closely coupled with the amount of low temperature reactions [66].

3.2.4 LTC Fuel Performance Index

The LTC index is a new metric developed for ranking the appropriateness of fuels in LTC engines based on the fraction of potential fuel savings obtained in the vehicle driving cycle [70]. The LTC index can be utilized to rank LTC fuels and predict their future performance. This index can also be used to recognize attractive fuels for LTC engines or assist in the development of new fuels for LTC engines.

The LTC fuel index is defined as the percentage of fuel savings obtained by HCCI operation and depicted by Eq. (3.19):

$$\begin{aligned} I_{\mathrm{LTC}} &= \frac{m_{fs,\,\mathrm{SI+HCCI}}}{m_{fs,\,\mathrm{HCCI}}} \times 100\% \\ &= \frac{m_{f,\,\mathrm{SI}\in\mathrm{HCCI}}}{m_{f,\,\mathrm{SI}}} \times 100\% \end{aligned} \tag{3.19}$$

where $m_{fs,\mathrm{SI+HCCI}}$ is the fuel consumed over the hybrid SI/HCCI operation, $\mathrm{m}_{\mathrm{fs,\,HCCI}}$ is the fuel savings for full HCCI operation, $m_{f,\mathrm{SI}\epsilon\mathrm{HCCI}}$ is the fuel consumed during the baseline SI operation over the possible HCCI operating range and $m_{f,\mathrm{SI}}$ is the baseline SI fuel consumption over the entire driving cycle. The LTC index (I_{LTC}) can also be understood as the mass-weighted percentage of discrete viable HCCI operating points [70]. The LTC fuel index combines information about the fuel operating region (the viable HCCI combustion engine loads and speeds) with the operating conditions required during engine operation at a particular real driving cycle.

3.3 LTC Fuel Design

The HCCI engine combustion is typically controlled by the reaction kinetics of different species present in fuel (Sect. 2.2.2 of Chap. 2). The chemical kinetics is governed by physical and chemical properties of fuel along with their spatial and time histories in the cylinder, which are dependent on engine design and operating parameters.

Generally, high cetane number fuels tend to extend lean-burn region in LTC engine due to higher fuel reactivity. Higher reactivity of high cetane fuels limits the high load operation at richer mixture due to advanced combustion phasing and excessive HRR. To overcome the problem of higher reactivity at higher engine loads, higher octane number (lower reactivity) fuels are used in LTC engines. Autoignition-resistant quality of high octane fuels prevents advanced combustion phasing at higher engine loads. The higher octane fuels face the challenge at lower load conditions as engine is operated on leaner fuel–air mixtures. The lean engine operation encounters misfire or partial burn cycles at lower intake temperature and load operations. Hence, cold start and lean-burn challenges are present in HCCI combustion using high octane number fuels. Additionally, various studies depicted that conventional fuels (diesel/gasoline) or pure single-component fuels are not able to fulfil the HCCI combustion requirements over a wide range of engine operating conditions [52]. Therefore, it is required to make fuels more suitable for HCCI combustion by reforming or designing the fuel's physical–chemical properties, fuel components and composition along with fuel molecular structure. Figure 3.16 illustrates a proposed HCCI fuel design concept.

The main challenge in HCCI engine is the control the ignition timings and HRR, to avoid the excessive noise and exhaust emissions. To achieve HCCI combustion over a wide range of engine operating conditions, reconfiguration of fuel properties and compositions is required for improving the adaptability and compatibility of various fuels [52]. All the approaches such as fuel additives, dual fuel engine operation, fuel blending and optimized fuel composition in real time can be utilized to redesign chemical properties of the charge based on HCCI engine load (Fig. 3.16).

Stratified charge compression ignition (SCCI) is proposed to enlarge the operating region of HCCI combustion engine (Sects. 2.4, 2.5 and 2.6 of Chap. 2). Typically, moderate inhomogeneities (temperature, air–fuel ratio and fuel composition) are required to obtain wider engine operating range, a smooth heat release, ignition timing controllability and lower emissions in LTC engines. Flexible control of combustion phasing using temperature stratification, fuel concentration stratification and fuel composition stratification can be utilized to achieve higher operating range, while maintaining higher maximum thermal efficiency and lower exhaust emissions. This target can be achieved by a combination of fuel design and fuel injection strategies. Figure 3.17 demonstrates the basic principle of fuel design and management in SCCI combustion engines.

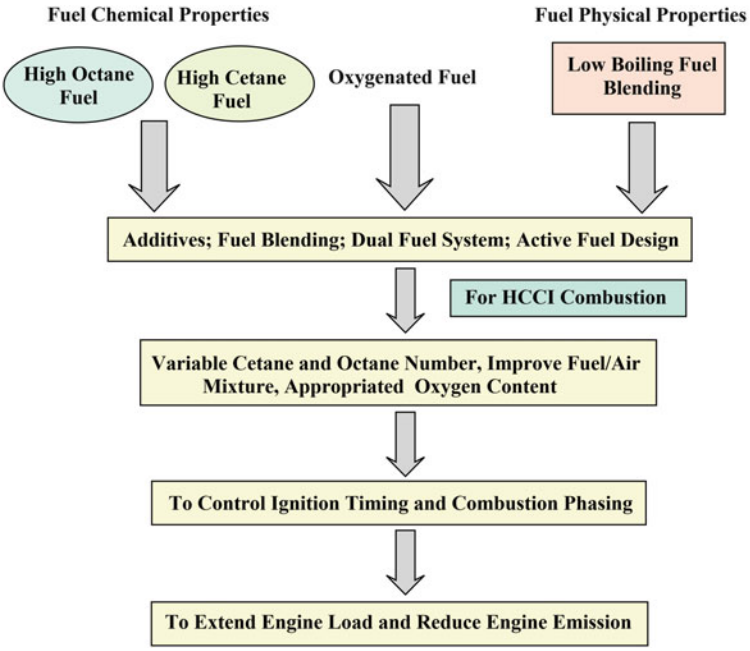


Fig. 3.16 Fuel design principles for HCCI combustion [52]

Figure 3.17 presents that in LTC engines, physical and chemical properties of fuels as well as fuel composition need to be managed actively on real-time basis depending on engine operating ranges. In advanced compression ignition engines, fuel concentration and composition stratification can be created using fuel injection strategies (PFI and DI) like in reactivity-controlled compression ignition (RCCI) and PPC engines. Test fuels can be selected with opposing chemical properties for port and direct injection, which can moderate the spatial local fuel–air composition distribution. Utilization of well-regulated controlled EGR is an effective method to control the HRR by reduction in combustion temperature [52].

3.4 Fuel Requirement in LTC Mode

Ideally any fuel can be used in HCCI engine by choosing the right design and operating conditions for autoignition of fuel–air mixture. In premixed charge compression ignition such as HCCI combustion, fully premixed fuel–air mixture is required before the start of combustion. The fuel must be volatile enough to allow sufficient mixing of fuel with air such that fuel-rich regions in the charge can be avoided to accomplish lower soot and NOx emissions. The simple method for homogeneous/premixed charge preparation is to inject the fuel in intake manifold

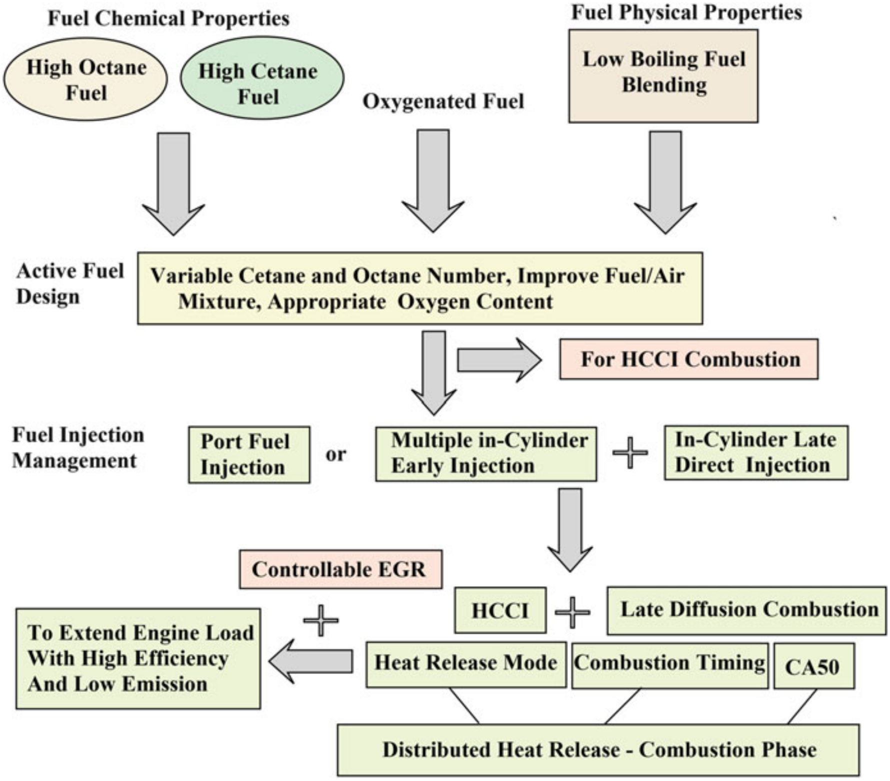


Fig. 3.17 SCCI combustion fuel design and management concept [52]

by port fuel injection (PFI) system. Fuel boiling point range plays an important role for using PFI system. The PFI works sufficiently well with gasoline-like fuels with boiling point up to 180 °C [2]. Gaseous fuels do not have issues related to mixing with port injection. Thus, most of the available high octane fuels can be used by PFI in LTC engines.

Fuels with lower volatility can use direct injection (DI) mixture preparation strategies by using high-pressure injection, multiple injection and improved injector design. Diesel has a high initial boiling point, and thus it will not evaporate and mix with air without intake preheating during PFI in the manifold. Diesel fuel is very difficult to use in HCCI engines using PFI system. A combination of low compression ratio and high intake temperature is required to use diesel in HCCI engine [38]. Minimum 100 ° C intake temperature is required to use high-boiling-point fuel (diesel). Thus, it is concluded that the high-boiling-point diesel-like fuels should not use PFI, and use direct injection system to obtain proper atomization and mixing. To prepare sufficiently premixed charge, early direct injection at comparatively lower injection pressure is used to obtain premixed charge in LTC engines.

Fuel autoignition quality is of critical importance in LTC engine due to the nature of ignition. The autoignition characteristics of fuels must satisfy the varying requirement of the engines over a wide range of operating conditions. On investigating wide ignition quality fuels in HCCI engines, it is summarized that ideal HCCI ignition quality for dedicated HCCI engines is in the range of CN 35–45 (approximately 70–50 RON, respectively) [25, 62, 71, 72]. Other LTC strategies, such as RCCI combustion, uses both high and low reactivity fuels.

The PPC combustion mode can be achieved with diesel fuel as well as high octane gasoline-like fuels [73]. At lower engine loads, diesel is a well-suited fuel, and at higher engine load, gasoline-like fuels are more suitable fuel for PPC mode operation. Ideally ON of PPC fuel should be a function of engine load. A study suggested a simple thumb rule for optimum fuel ON as a function of engine load. The optimum ON is five times the load in indicated mean effective pressure (IMEP). This indicates that the fuel can be very similar to diesel at idle engine operating conditions, and at full engine load conditions, an ON of 100 or higher is required for the desired performance of the engine.

The charge preparation and autoignition control strategies in LTC engine for different automotive fuels are discussed in Chaps. 4 and 5, respectively.

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