

Prospects of Hydrogen in HCCI Engines-A Review

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Abstract

Automotive engines have been running for years with conventional or petroleum derived fuels (gasoline or diesel). Scarcely few automobiles have been using gaseous fuels such as liquified petroleum gas (LPG) or compressed natural gas (CNG). Over the years, large scale use of conventional type of combustion engines namely spark ignition and compression engine with petroleum derived fuels has led to high rise in greenhouse gases with major being carbon dioxide. To circumvent the problem of automotive pollution, non-carbon or low carbon fuels are being encouraged. In this direction, hydrogen being high energy carrier is a good candidate for use in automobiles. Thus, hydrogen has been explored as an alternate fuel due to its good properties but resulted in high NO_x emissions. Also, in the advent of new combustion processes, a novel combustion process combining the good features of conventional combustion process is gaining increasing attention from combustion community. In this regard, homogeneous charge compression ignition (HCCI) engine concept has been evolved. HCCI mode derives good features of conventional engines yielding simultaneous reduction of NO_x and particulate emissions. Even much more benefits can be extracted with the use of hydrogen in HCCI mode of operation. In spite of its good features, HCCI opens challenges in terms of uncontrolled auto-ignition, high peak pressures and poor high load capability. Through, present review work, it is observed that many techniques are explored to achieve HCCI mode of operation and apart from experimental studies, multi-dimensional modelling works revealed much insights into its behaviour. Swirl along with other pertinent engine operating parameters could address challenges to a significant extent. Biomass resources are being seen as potential sources for production of hydrogen. Addition of hydrogen, with fuels such as DME, diesel, and bio-fuels could reduce harmful emissions substantially without any penalty on engine performance compared to its use in neat form.

Keywords: Hydrogen, Renewable, HCCI Engine, External mixture formation, Swirl, NO_x-PM Emissions

1. Introduction

Internal Combustion Engines have been serving the mankind for the past about 150 years with fuels mostly derived from fossil reserves-petroleum fuels. The dependence on fossil fuel run vehicles is so much that it is beyond imagination to think

of a life without such prime movers. Also, these fossil sources are serving to meet energy requirements and production. The exponential growth in the vehicular population has also increased fuel sources. The vehicle development also expanded other sector in the event of civilization and massive urbanization. While these are the merits and the limitations. Being increased air pollution due to vehicle population. The fossil reserves have been concentrated in certain pockets of planet and has brought huge wealth to one strata and nations which have limited sources have been heavily dependent on rich nations and hence losing hard earned revenue. The limited reserves of fossil fuels rising doubts of its availability. To tackle the issues of sustainability and ecology related issues, researchers have venturing into alternative fuels derived from petroleum sources and also non-petroleum sources such as renewable sources. To achieve, energy independence it is a good option to choose fuels from renewables such as bio-resources. In this regard, each alternative fuel has its own advantages and limitations. However, certain bio-resource fuels are having carbon in its structure and therefore it is good look for non-carbon and renewable source related fuels. This aspect paves way for use of Hydrogen, an energy carrier, could be good option. In its simplest form has lowest atomic mass and combines with life giving oxygen to yield another important product without which existence is of life is impossible. As one goes into its origin it derived its name from Latin word-“hydrogenium,” with two Greek words hydro and genes (i.e.water and forming) credited to its inventor- Henry Cavendish observed that the gas was flammable and when combusted produced water and thus described it as “flammable air”. It finds first place in Mendeleev’s periodic table with the symbol H [1].

Owing to its high heating value and being a gas, which gets quickly atomized, could be good option as an alternative fuel with no carbon in its structure and thus no carbon related emissions, especially CO₂ when combusted. The beauty of hydrogen production is that its oxidized product is its source of production. Since the basic method of obtaining it is from water, its wide use greatly reduces dependence on other nations. The efforts of researchers are not confined to search for finding sustainable and viable fuels but also to developing alternative engine combustion systems different from conventional SI and CI versions. Among these, rotary combustion engines, stratified charge engines, lean burn engines [2]. Hydrogen as energy carrier possess excellent thermo-physical and combustion properties to suit to the existing engine technology with few modifications. Due to its

good combustive properties and releases only, water molecule when combusted with oxygen and hence be the cleanest fuel. In the event of developing new combustion process, the hybrid combustion process has emerged combining the features of conventional SI and CI combustion called Homogeneous Charge Compression Ignition (HCCI), has gained wide acceptance by combustion community [3]. Unlike, fossil fuels, hydrogen is a manmade fuel and not a naturally occurring and need to be generated and hence expensive compared to petroleum derived fuels. Hydrogen is no doubt a good alternative fuel candidate in combustion engines, however, it has been also explored in fuel cells especially in Proton Exchange Membrane Fuel cell (PEMFC) which can operate relatively at lower temperatures compared to other fuel cell types [4]. Whereas for vehicle fuel cells the study focuses on performances, cost, infrastructure, type of storage and type of productions in hydrogen. Exploring any fuel as alternative to fossil fuel, besides aiming for better performance and low emissions it is highly desirable to look into the aspects to be viable, safe on-board storage, economical cost of production and storage and safety of operation are to be considered. The essential feature of HCCI concept is that it simultaneously reduces particulate and NO_x emissions. Many a researcher have adopted hydrogen either as sole fuel or in blended with other fuels to improve the performance and reduce the emission burden [5-10].

The present paper reviews the works carried out on the use of a high energy carrier hydrogen in HCCI engine so that the advantages good fuel and hybrid combustion can further be gained in addition outlines briefly the properties, the production, and engine characteristics when hydrogen is used in HCCI mode of operation.

2. Suitability of Hydrogen as a fuel in combustion engines

A thermodynamics or combustion related engineer aims at thermo-physical, combustion properties besides its anti-knocking tendency and reliable operation, safety of operation and production costs plant, acceptability of hydrogen fuelling station and life cycle of hydrogen [11,12]. Due to its high auto-ignition temperature, the hydrogen has long been explored in spark ignited engine by blending, injecting either directly into cylinder or intake manifold [13]:

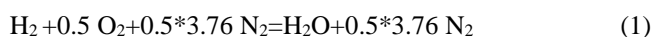
2.1. Thermo-physical and Combustion properties of hydrogen

Among the elements seen in periodic table, hydrogen exists with lowest atomic mass and being a gas occupies large volume and hence it is required to be liquified at cryogenic temperatures and stored in containers which do not get corroded and embrittled. Hydrogen, a non-odorous, is a highly flammable gas which can be easily miscible with air and burns without a visible flame. Hydrogen flame being non-luminous is thus free from particulate emission but raises a concern with regards to safety of operation and storage. The important properties- ignition energy, limits of flammability, anti-knocking property (octane number) have been widely investigated for its development as a fuel in hydrogen run

vehicles, are listed in Table -1. Works related with its use as a fuel and its properties are compared with iso-octane and methane, which are representing as the natural gas and gasoline, respectively [14-16].

Molecular weight(g/mol)	2.016
Density(kg/m ³)	0.08
Auto-ignition temperature in air (K)	858
Minimum ignition energy (mJ)	0.02
Minimum quenching distance (mm)	0.64
Flammability limits in air(vol%)	4-75
Lower heating value (MJ/kg)	120
Octane rating	>120
Burning velocity(m/s)	1.85
Stoichiometric air-fuel ratio(kg/kg)	34.32:1
Adiabatic flame temperature (K)	~2400

For any fuel to be used in engines, firstly stoichiometric or theoretical or chemically correct amount of oxidizer required for its complete combustion is determined. For engine of practical use, normally air will be oxidizer and typically atmospheric air consists of 79% and 21% by volume of nitrogen and oxygen respectively. This necessitates that for every one mole of oxygen O₂, 3.76 moles of nitrogen N₂ enters the combustion chamber [9,11]. Therefore, for combustion to be complete, only H₂O forms with N₂ left unreacted, as shown in Eq.1.



Therefore,

$$\text{Air/Fuel ratio} = \frac{(0.5 * 32 + 0.5 * 3.76 * 28)}{(16 + 52.64)} = \frac{68.64}{2} = 34.32:1 \quad (2)$$

This gives an information that for complete combustion of hydrogen with air, each part of hydrogen is to be allowed to reacts with 34.32 parts of air. For a typical petroleum fuels except methane, in general, the theoretical A/F ratio is 15:1(approx..). Hence, theoretically speaking hydrogen demands double the amount of air required for complete combustion, relative conventional fuels. This states that the size of engine cylinder should be larger enough to accommodate such a fuel.

Since the engine operates not always with stoichiometric ratio and owing to high heating value and wide flammability limits of hydrogen, it thus reacts and releases very high temperatures. This high temperature makes inert nitrogen to get dissociated into atomic nitrogen and under favourable conditions, it splits molecular oxygen into atomic oxygen and thus the radicals (N and O) forms rapidly complex compounds of oxides of nitrogen (mostly NO, N₂O and NO₂) and thus denoted as NO_x.

Therefore, nitrogen oxides are formed in bulk with combustion of hydrogen, a undesirable phenomenon and over the years researchers have been tackling the issue of minimizing the release of NOx emissions with combustion of hydrogen.

It can be seen from Table-1, that the flammability limits of hydrogen-air mixture are at 4–75%, indicating wide range of flammability as compared to other fuels and moreover, it represents amount fuel/ oxidizer requirements and it can be realized that hydrogen could work in rich and lean conditions and for economizing fuel, lean mixtures are preferred and thereby necessitating complete combustion [16,17].

The burning velocity is a function of equivalence ratio and thus be altered with regulation in equivalence ratio. Its values for hydrogen-air mixtures are about 0.12 m/s (at $\phi=0.25$) and 3m/s (at $\phi=1$) respectively, far high compared to gasoline-air mixtures. This in turn related to emissions such as NOx [18].

Hydrogen's minimum ignition energy and quenching distance are small compared to mixtures of iso-octane–air. This raises concerns with respect pre-ignition due to hot spots and thus with minimum ignition energy, the hot spots allow burning without a spark plug. However, quenching distance allows flame extinguished. For engines, among the sources of pre-ignition include, high temperature components, hot spark plug areas, exhaust valves and hot spots, trapped gases and crevice

regions [13,20].

On the other hand, hydrogen's high auto-ignition temperature, which much higher than most of fossil fuel-air mixture and permits to go for a high compression ratio compression ignition engine or its use is limited spark ignited engines. Due to low density of hydrogen, it needs to be stored in large and number of containers or be liquified to cryogenic temperatures and then be stored in cryo-containers making its storage a cost intensive, for providing enough power and range as with other fuels [19,20].

In addition, with very high diffusivity of hydrogen, it disperses faster in air more than commonly used fuels such as methane and iso-octane. Due to these characteristics added with high heating value, hydrogen fuelled engine are more prone for undesirable phenomena such as abnormal combustion and pre-ignition [21,22].

The high diffusivity characteristic of hydrogen makes it to propagate backwards leading to undesirable phenomena such as flashback or backfire due to which the flame traverses back into its storage and is an uncontrolled and highly hazardous and many studies have been done in using flame arrestors and flash traps [23]. The high octane rating of hydrogen allows it with stand detrimental effects of knock if parameters affecting are properly controlled [25].

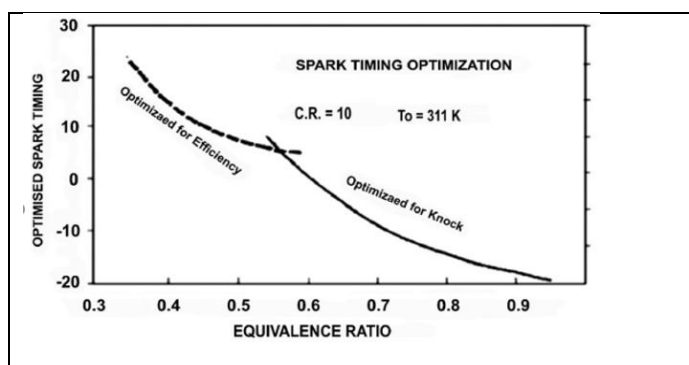


Fig.1 Variation of spark timing with equivalence ratio giving limits efficiency and knock for hydrogen [7]

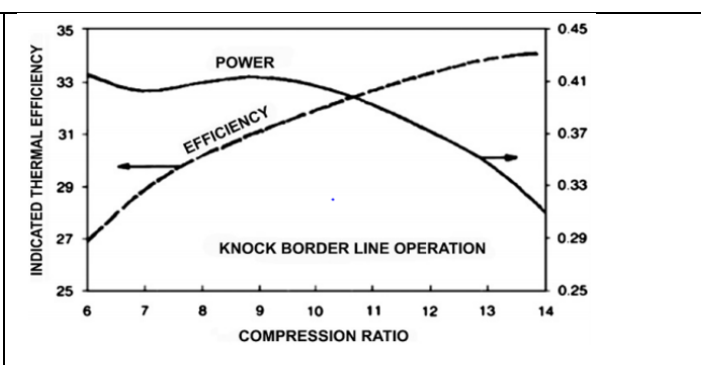


Fig. 2 Variation of indicated efficiency with compression ratio for knock free operation limits for power and efficiency [7]

Figs. 1 and 2 gives the optimized spark timing and knock free operation limits when operated under varying equivalence ratios and compression ratios respectively [26,27]. Thorough control of fuel-to-air equivalence ratio is essential to avoid abnormal combustion with hydrogen run operation. As hydrogen's flammability permits to with wide mixture strengths, it is optimum to work with lean mixtures thereby adopting lean-burn strategy for reducing component as well as combustion temperature.

Techniques such as water injection and exhaust gas recirculation (EGR) have been used to overcome pre-ignition difficulties and also to limit peak combustion temperature thereby controlling NOx emissions. Different proportions of residual gases have circulated as thermal dilution to a maximum of 30% of its fresh charge capacity to reduce undesirable effects due to back fire [28].

Certain materials are sensitive for handling hydrogen, if proper care is not taken in selection of mechanical properties of storage tanks, embrittlement occurs mostly with iron. Materials such as brass and copper alloys, aluminium and aluminium alloys, and copper beryllium are good choice for handling hydrogen whereas nickel and high-nickel alloys, titanium and titanium alloys are very sensitive to hydrogen embrittlement [15, 29]. For use of hydrogen with steel, proper composition is essential to avoid hydrogen embrittlement [30].

The air-standard or thermodynamic efficiency of an Otto cycle-based engine is related to compression ratio of the engine and ratio of specific heats, as shown in Eq.3.

$$\eta_{th} = 1 - \left(\frac{1}{r^{\gamma}}\right)^{\gamma-1} \quad (3)$$

Therefore, air-standard cycle efficiency is a simply a function

of compression ratio r_c and the specific heat ratio γ . In practice, it's not such simple, it depends on several other factors [2].

2.2 Engine performance and emissions with hydrogen as a fuel:

Power developed by the engine with hydrogen mainly depends on the factors such its low density, heating value and conditions of operation leading to pre-ignition. Hence, to overcome problem with low density and thereby poor volumetric efficiency under naturally aspirated conditions, studies have

been done to use it effectively by supercharging. Al-Baghdadi [6] in their numerical and experimental study, employed supercharging by varying certain pertinent parameters for improving the performance and reduction of NOx emission of a four-stroke hydrogen fuelled engine.

Based on their experiments on a Ricardo E6/US engine, they developed a chart indicating the safe operation zone without pre-ignition, acceptable NOx emission, engine efficiency and lower specific fuel consumption in comparison with the gasoline engine.

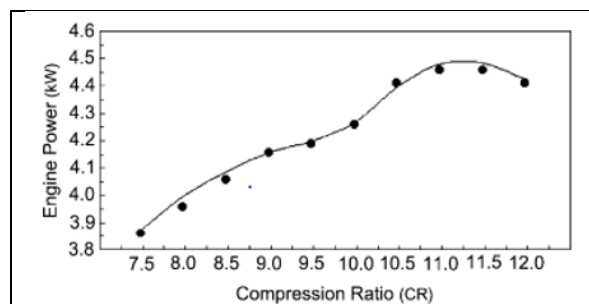


Fig.3 Comparison of experimental and prediction on the effect of compression ratio on engine power with hydrogen fuelled naturally aspirated engine [6].

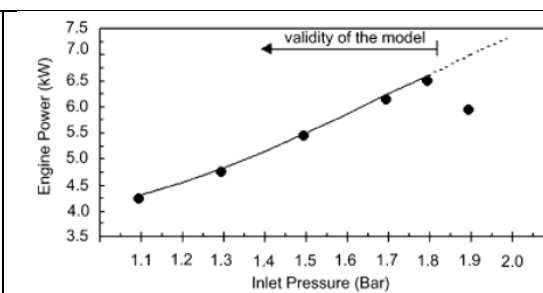


Fig.4 Comparison of experimental and prediction on the effect of inlet pressure on engine power with hydrogen fuelled engine [6].

Due to high stoichiometric air-fuel ratio requirement with hydrogen operation, engines of larger with turbochargers or superchargers than usual gasoline are required. They were of opinion that supercharging is to be preferred over choice of high compression ratios [34].

Hydrogen being a gas, gets easily atomized and free from carbon hence produces non-carbon related emissions hence it is considered as an ideal alternative fuel to hydrocarbon fuels and only potential emissions from hydrogen fuel run engines were NOx emissions [31,32].

Hydrogen has very high heat value and with operational range of fuel-air ratio and engine speed, very high combustion temperatures are realized and favourable conditions for formation of NOx emission will take place [33]. However, in the process of reducing NOx emissions the parameters such as varying spark timing, thermal dilution by exhaust gas recirculation, varying injection timing, varying compression ratios and engine speed have been employed [2,3,5].

2.3 Production of Hydrogen:

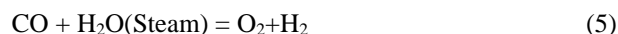
World over there are many sources which are abundant for production of hydrogen in the world.

Water electrolysis has been widely employed for stationary and on-board applications. Among electrolysis, methods such as alkaline water electrolysis, water electrolysis and high temperature electrolysis have been used for production [35].

As biomass is widely available and moreover it is renewable source, methods have been suggested for generation of

hydrogen from various kinds of biomass and commonly used technique is biomass gasification. Though there are various methods available for production of hydrogen, the final choice lies on the availability of large resources, feasibility of production and cost of storage and environmentally safe [12]. Plant and animal wastes are being used for obtaining biomass. Most commonly fuels produced from biomass are methane, bio-gas, syn gas and producer gas. However, production of methane has been largely explored as it has good and high heating value, with single carbon in its structure and with high hydrogen-to-carbon ratio. Methane could also be produced from bio-gas and stored in a compressed form. Hydrogen on a large scale been produced from steam reforming method.

Basically, it is a method of hydrolysis of methane under high temperature -steam. In the stream of high temperature steam, the hydrogen atoms separate from the carbons atoms in methane (CH₄), is an endothermic reaction. The reaction involved in steam reforming are as under:, which is the reaction that consumes heat to produce synthetic gases as H₂ and CO.



To obtain synthesis or syn gas, finely crushed coal(pulverized) is allowed mix with oxidant at high temperature around 2000 °C. The typical constituents of synthesis gas are carbon monoxide, hydrogen and traces of sulphur related gases. The process should be made commercialized and viable to substantially replace conventional fuels [36].

Though in experimental stage, hydrogen is being produced from photo catalytic water splitting making use of renewable

energy sources such as solar energy instead using conventional power source [37].

In addition to solid oxide electrolysis, techniques such as alkaline water electrolysis, polymer electrolyte membrane (PEM) electrolysis are available for production of hydrogen. The source of power required to carry out the electrolysis, the constructions, conversion efficiency, and availability in industries are factors that makes difference among various methods of electrolysis. [38-40]. Photo-electrolysis is newly evolving area making use of solar energy works with high efficiency [41].

Similar to Photo-electrolysis, the process makes use of light energy for dissociating water into its constituents-hydrogen and oxygen is called Photolytic process and is presently in nascent stage of its research and development and in addition two new processes have come up viz photobiological water splitting and photoelectrochemical water splitting.

3. Description of HCCI Engine:

Homogeneous mixture of air and fuel is prepared in a conventional SI engine and ignited with a spark at the end of compression whereas air alone is compressed to a self-ignition temperature of fuel in a CI engine and due to heterogeneous mixture formation, the combustion is initiated. As mixture of fuel and air participates initially, in a SI engine, the throttling makes lower fuel efficiency, however, due to precise injection of fuel, CI engine delivers relatively better performance but

with higher NO_x and PM emissions. HCCI engine combines the good features of conventional SI and CI engine with homogeneous mixture of fuel and air participates in combustion initiated by auto-ignition due to compression alone [3]. Fig. 5 illustrates the comparison of different modes of combustion.

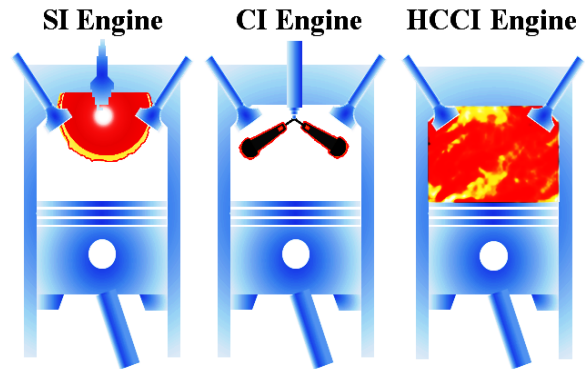


Fig.5 Illustration of SI, CI and HCCI combustion processes.

Thus, HCCI concept is predominant with temperature and mixture strength, a chart is developed to show the interaction of temperature and equivalence ratio with regimes depicted with soot and NO_x formation under the interaction these two parameters, as depicted in Fig.6.

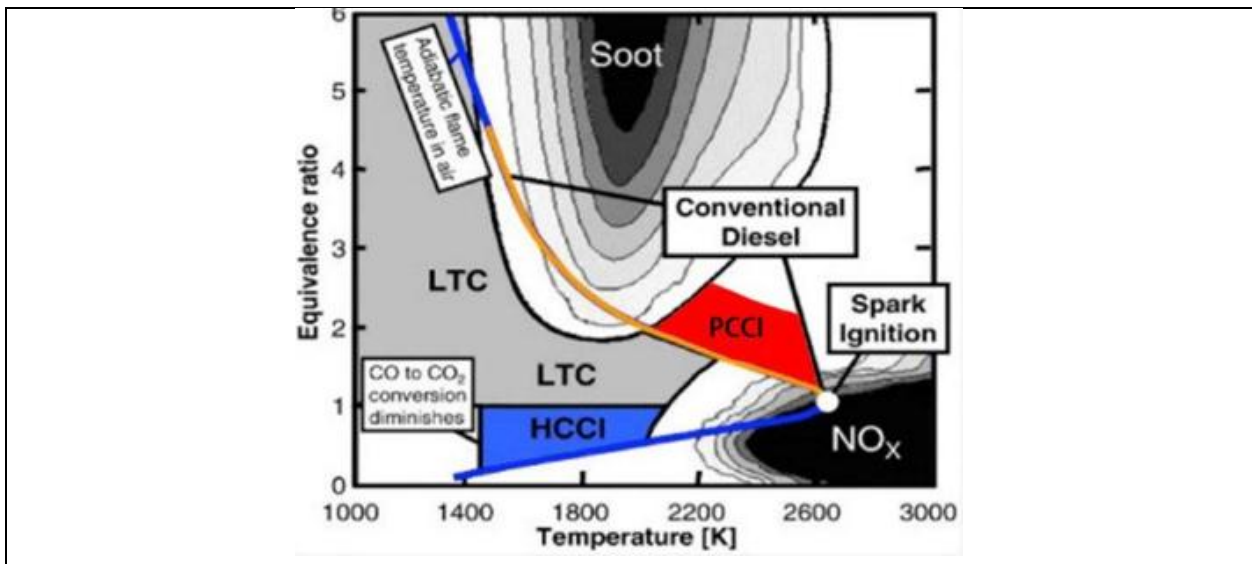


Fig.6 Variation of equivalence ratio with temperature depicting regions of different combustion processes [Xingyu Liang, Zhiwei Zheng, Hongsheng Zhang, Yuesen Wang and Hanzhengnan Yu A Review of Early Injection Strategy in Premixed Combustion Engines Appl. Sci. 2019, 9(18), 3737 <https://doi.org/10.3390/app9183737>].

The process adopted in HCCI has derived two more sub-concepts viz premixed charge compression ignition (PCCI) and reactive charge compression ignition (RCCI). Basically, HCCI works with auto-ignition and is mostly regulated by chemical kinetics and operates under lean mixtures with spontaneous

ignition and volumetric combustion take place under low temperatures without a flame propagation and thus yields good fuel efficiency and simultaneous reduction in NO_x and PM emissions, and accommodates variety of fuels [4, 42-45]. Auto-ignition is highly uncontrolled phenomenon and hence HCCI

combustion leads to new challenges with respect to high peak pressure, difficulty in cold-start and poor full-load capability [46-47]. About 15% reduction of fuel consumption was reported by General Motors (GM) with their new prototype gasoline HCCI engine car [48]. Though HCCI appears to be attractive, earlier studies revealed low specific output, narrow operating range, uncontrolled auto-ignition, long start-up time and high CO and UHC emissions [49,50].

No visible flame propagation was observed in HCCI mode of combustion establishing volumetric combustion of HCCI engines [51-54] aided by flow visualization studies with Schlieren photography, Particulate Image Velocimetry (PIV) and Laser Doppler techniques. Even though there are various ways achieving HCCI combustion, all methods are generally categorized in to two broad methods, as represented in Fig.7.

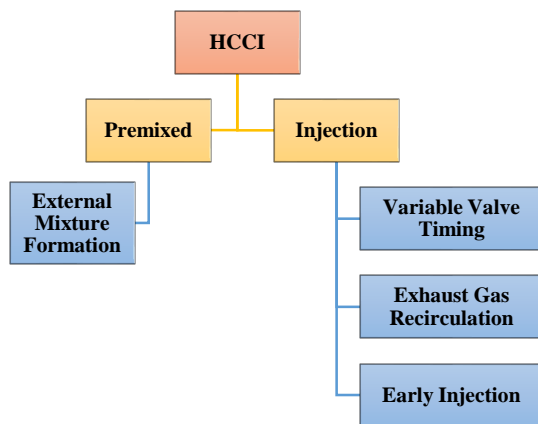


Fig.7. Techniques to achieve HCCI mode of operation.

3.1 Premixed type:

This type combines the features of SI and CI engines with intake of lean mixtures accompanied with high compression ratio but without any external source of ignition and hence relatively low temperatures are attained leading explosion of inducted charge attaining volumetric combustion releasing low NOx and soot emissions but with high CO and HC emissions.

A technique called external mixture formation has been followed to achieve premixed mode of HCCI combustion where in vaporized fuel mixed with air enters the combustion chamber. This technique successfully achieved however deteriorated engine's indicated specific fuel consumption relative to conventional mode of combustion engines [55,56].

3.2 Injection type:

In this type conventional CI method of allowing fuel and air mixing and following certain operational changes the way the mixing is permitted with residual gases to achieve HCCI mode of operation. One of the methods is to adopt negative valve overlap (NVO) to significantly reduce NOx emissions, instead of permitting external exhaust gas recirculation, with a sole objective to obtain HCCI mode of combustion. By this method, internally available residual gases before their escape would help mix with incoming fresh charge and aids in auto-ignition

along with possible better thermal stratification [57-60]. Both external EGR and NVO methods have undoubtedly yielded reduction in NOx emissions with a penalty on net power [61-63].

Among the methods of variable valve timings, early exhaust valve closing (EEVC), early inlet valve opening (EIVO) were followed to achieve HCCI mode of operation. However, early injection led to higher CO and HC emissions due to adherence of fuel and poor scavenging though permitted to obtain HCCI mode of operation [64,65].

3.3. Numerical studies on HCCI engines:

Even though experimental methods have permitted to obtain insights into behaviour of engine pertain to its performance parameters and emission characteristics in HCCI mode of operation, computer simulations allow to include all possible parameters to arrive at an optimal solution. This is a good attempt since the engine's actual combustion is more complex and moreover HCCI combustion is still a vigorous exercise to conduct extensive experimentation.

In this direction, researchers have written in-house codes or making use of commercially available software. The software simulations have paved the way better understanding of complex nature of HCCI concept both for single cylinder and multi-cylinder engines. Multi-dimensional models using KIVA, AVL-FIRE, STAR-CD and ANSYS-FLUENT combined with CHEMIKIN, have attracted many a combustion community and yielded good results.

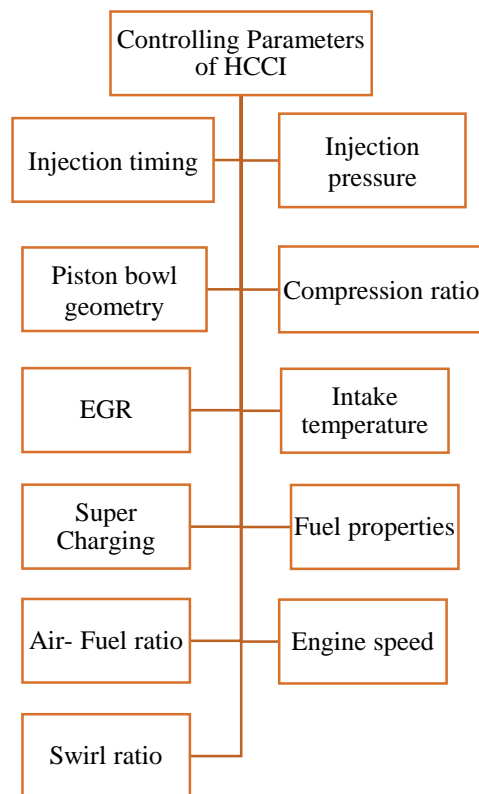


Fig.8. Parameters that affect the performance of the HCCI engine.

Sharma et al. [64] considered various engine's geometrical, operational parameters and fuel properties affecting typical engine's performance and emissions, were considered in HCCI mode operation by following external mixture formation. The controlling parameters are depicted in Fig.8. The parameters were selected to address and overcome the challenges faced in achieving HCCI mode of combustion.

Effect of swirl ratio has been considered as a pertinent parameter and linked with the parameters listed in Fig.8. They did computer simulations with the help of STAR-CD software for relating the interdependence of listed parameters. They considered the engine geometry and method of external mixture formation studied by Ganesh et al. [56]. They also extracted contours of turbulent kinetic energy and velocity magnitudes for different parameters studied. They concluded that swirl has significant effect on the HCCI engine performance and emissions and observed reduction peak pressures, temperatures and CO₂ and NO_x emissions with a marginal reduction in power. Even though increase in wall heat transfer losses has been noticed but significant reduction in CO and NO_x emissions were seen with the combined effect of EGR and swirl. Within a selected range of lean mixture strength (0.26-0.86), an equivalence ratio of 0.46 has been optimized, for the chosen engine configuration, with better engine performance.

4. Fuels for HCCI engines-Hydrogen:

Variety of fuels, which can easily be vaporized and mixed with the air before ignition, have been tried out in HCCI engines [66]. Fuels such as alcohols, n-heptane, iso-octane, hydrogen, etc. with varied auto-ignition points have been used.

To ease the mixture formation different fuels, effect of increased intake temperature for auto-ignition at different compression ratios has been studied for attaining HCCI operation [66]. With high compression ratios and fuels of high-auto ignition temperature knocking or misfiring were avoided. In HCCI mode, Antunes et al. [67] observed increase in IMEP with decrease in air intake temperature. To observe load range and knock characteristic with HCCI mode, studies were done at high loads [77]. Many a researcher have used hydrogen as an additive either to improve engine performance or to control ignition timing, as it highly unstable as single fuel [69-72]. Increase in engine efficiency and marginally low emissions were obtained when hydrogen is blended with natural gas in a diesel engine in CI and HCCI modes [72-75]. Moreover, many bio-fuels such various vegetable oils, were used in non-HCCI mode, have been used along with hydrogen to improve engine performance [76]. Due to high heating value and high diffusivity of hydrogen, mixes quickly with air, could be right choice as a sole fuel but engine operation would be unstable and knock prone [74,78]. Therefore, a combination of both (high cetane number fuels and high-octane number fuels) provides soft engine run [74], whereby the mixture can be operated at high CR and has longer combustion duration. Owing to hydrogen's wide flammability limits, it can work wide mixture strengths and develop wide range of engine power outputs [75].

HCCI with good lean mixture working, develop high brake thermal efficiency [56], showing that hydrogen is able to operate with extremely lean mixtures and still maintain a relatively high efficiency compared to conventional diesel fuelled CI engines. Partially premixed charge compression ignition PPCCI instead of HCCI, is different in injection methods meeting the basic purpose of obtaining a homogeneous mixture.

4.1 Emissions with hydrogen as a fuel:

As HCCI engine mode of operation is aimed at achieving simultaneous reduction in PM and NO_x emissions, but has led to higher UHC and CO emissions in HCCI engines relative to conventional diesel engines [56,67,79]. However, tackling HC and CO emissions is easier with the provision of catalytic converter. With hydrogen as fuel, levels of NO_x emissions are observed to be lower than neat CI mode of operation [67]. With the use of hydrogen, except NO_x and no carbon related emissions were produced [75].

Studies by Miller and Bowman reported that NO_x emission in the close vicinity of stoichiometric mixture is dominant by thermal mechanism where as in lean side Fenimore mechanism is prevalent [80]. Use of high compression ratios would reduce NO_x emissions in HCCI engines and would further be reduced with high higher fractions of EGR [81,82], as EGR would reduce effective amount of oxygen taking part in combustion but with increased HC and CO emissions. To reduce both NO_x and CO emissions, internal hot high pressure EGR with variable valve timing were utilized [83]. High pressure injection and high air-fuel ration enable good atomization would finally reduce PM emissions and would further be reduced with the addition of hydrogen [84,85].

Hydrogen at best be produced from renewable sources such as biomass and could be good choice for engine as a sole fuel or in blended form but its use in existing CI engine be improved by employing higher compression ratio due to high auto-ignition temperature of hydrogen and handling of hydrogen in terms of difficulties such as frostbite, suffocation, embrittlement, component failures and explosion [86-90].

Requirement of homogeneous mixture of fuel and air is essential and can be better achieved through the use of hydrogen and observed to yield high efficiency and moreover hydrogen at best be produced on-board. Also, with increased quantity of hydrogen, reduced auto-ignition time and increased peak pressures and indicated power were achieved [91-93]. Addition of hydrogen is good but beyond a certain amount in terms of energy ratios of two fuels is to be limited to reduce knock occurrence and NO_x levels as revealed by Szwaja and Grab-Logarinski [94].

Through high speed chemiluminescence imaging, Persson et al. [95] studied the early flame development in spark assisted HCCI combustion by employing EGR and regulation of negative valve overlap.

Gomes Antunes et al. [96] utilized hydrogen as fuel in conventional CI and tried to operate in HCCI mode of operation by external mixture formation technique. They pre-heated the

air for allowing better mixing and to have controlled auto-ignition. They obtained high fuel efficiency with very lean air-fuel mixtures and obtained low NO_x and other emissions and observed power obtained is related to inlet air heating. They also noticed mechanically unstable operation and high peak pressures in HCCI mode of operation compared to conventional diesel engine mode.

Alias et al. [97] listed out the advantages of HCCI concept to lower the emissions and opined that it can handle wide variety of fuels gasoline, diesel, biofuels, and hydrogen and may emerge as a futuristic scope for achieving commercialization of concept. They concluded that HCCI mode would give better results with combination of hydrogen with biofuels. Namar and Omid [98] did numerical studies on engine's performance by conducting energy and exergy analysis of a hydrogen-fuelled HCCI engine. They developed a single-zone thermodynamic model with detailed chemical kinetics and concluded that pressure at inlet valve closing (IVC) and equivalence ratio had prominent effect on irreversibility and exergy terms whereas engine speed has minimal effect on irreversibility production. Also, power, irreversibility and engine volumetric efficiency were closely related to IVC pressure and temperature enhancement which in turn affect the chemical exergy.

Pochet et al. [99] experimentally investigated the use of ammonia-a high-density hydrogen carrier as a fuel in HCCI engine. They have done engine test bench with a compression ratio of 22:1 and inferred that with the use of lean mixtures and EGR, even fuel borne NO_x emissions were reduced significantly. Caton and Pruitt [100] did both numerical and experimental work on a hydrogen fuelled HCCI engine using a single-zone model based on chemical reaction kinetics and using a single-cylinder Cooperative Fuels Research (CFR) diesel engine respectively. They employed intake heating and lean mixtures and observed low NO_x emissions even with a comparable diesel engine operation. They inferred that engine's surface area-volume ratio could be a factor for higher thermal losses and higher chemical enthalpy losses and lower efficiency of hydrogen run HCCI engine.

Stenlaas et al.[101] carried out experimental investigation of hydrogen as HCCI engine fuel. They compared HCCI and SI mode of operation. For obtaining HCCI mode operation the parameters adjusted were excess air ratio-lambda (λ), engine speed, compression ratio and intake temperature. They observed poor load ability in HCCI mode of operation compared to SI mode, however superior values of indicated thermal efficiency. Excess air ratio (λ) was observed to be a dominant factor in making HCCI operation feasible and obtaining lower NO_x emissions, much lower than with conventional SI engine operation.

Rosati and Aleiferis [102] carried out experiments on a single cylinder research engine equipped with both Port Fuel Injection (PFI) and Direct Injection (DI) systems with an optical access to observe in-cylinder phenomena. They concluded that backfiring and air displacement from hydrogen's low density were avoided with direct injection of hydrogen after intake valve closure. Full hydrogen fuelling HCCI was finally achieved even at the low compression ratio in line with air-pre-heating and negative valve overlap to promote internal EGR.

Zhao and Luo [103] in their review concluded that HCCI mode of operation with hydrogen be promoted as a fuel for effectively reducing the harmful emissions from combustion engine. Narioka et al. [104] observed improved fuel economy in HCCI mode of operation with hydrogen and DME when compared to HCCI operation with pure DME. They further concluded that by increasing the compression ratio, the amount of DME addition could be reduced with similar benefit in reduction of NO_x and HC emissions.

Hairuddin et al. [105] reviewed the experimental techniques and simulation methods adopted to use hydrogen and natural gas in HCCI Engines. They listed out specific strategies used in the experimental methods. They opined that when hydrogen is combined with diesel in dual-fuel mode, low NO_x, CO and particulate matter (PM) emissions levels could be obtained with increased engine efficiency reduced emissions levels but with reduced power. They recommended multi-zone simulation modelling methods to obtain insights to in-cylinder phenomena.

Ibrahim and Ramesh [106] in their paper compared results obtained by conducting experiments on a stationary engine in three different modes of operation, namely, hydrogen-fuelled HCCI (HHCCI), hydrogen diesel HCCI (HDHCCI), and neat diesel compression ignition (CI). They observed better thermal efficiency and low NO emissions by maintaining lowest charge temperature without misfire and best combustion phasing in HHCCI mode compared to conventional diesel mode. They observed smooth operation, without heating the intake charge, under hydrogen diesel HCCI mode (HDHCCI) to the extent of BMEP of 4 bar. They finally concluded that the HHCCI mode is promising in terms of thermal efficiency and low emissions.

Raitanapaibule and Aung [107] investigated numerically by CHEMKIN software 4.0, characteristics of HCCI engines fuelled with Methane and Hydrogen, For the purpose of simulation studies the effect of increasing the initial concentrations of H₂, varying the inlet temperature and equivalence ratio were incorporated. They concluded that with hydrogen addition, indicated power, peak temperature and pressure were increased, whereas ignition delay time decreased.

Hu et al. [108] carried out numerical studies using zero-dimension, single-zone thermodynamic model for analysing the effect of the auto-ignition characteristics of dimethyl ether (DME)/H₂/Air blends (with wide hydrogen blending ratio) HCCI engine. A two-stage heat release phenomenon at different crank angles was observed for all the mixtures simulated. They noticed retarded auto-ignition timing of DME in HCCI combustion engine with the hydrogen addition. Also, with the hydrogen addition, ignition timing at low temperature is retarded moderately whereas it delayed significantly at high temperature due to the increased negative temperature coefficient duration.

Abdul Khalif et al.[109] carried out an energy-exergy analysis combining first and second laws of thermodynamics to investigate the effects of percent excess air and ambient temperature on the hydrogen-fuelled homogeneous charge compression ignition engine. They did analysis for different ranges of excess air at an ambient temperature. They calculated

first law and second law efficiencies.

Bae[110] listed out advantages and limitations of engine operation in HCCI mode of operation. An experiment on dual-fuel HCCI operation with dimethyl ether (DME)/liquefied petroleum gas (LPG)/gasoline/hydrogen was presented. He observed propane was a more effective way to increase IMEP, and concluded that LPG as an ignition inhibitor, higher load limit was extended in a DME fuelled HCCI engine.

Wang et al. [111] emphasized the need of ignition timing control in HCCI engines. They adopted multi-zone model with CHEMKIN for predicting chemical kinetics of methane blending hydrogen. The ignition timing could be regulated by adjusting the hydrogen addition and EGR rate, for obtaining low emission levels. They observed that NO_x is mostly formed in core zones while HC and CO originated in the crevice and the quench layer and predicated that OH radical plays an important role in the oxidation.

Li et al. [112] studied both experimentally and numerically on the effect negative valve overlap in HCCI engine fuelled with natural gas and hydrogen by varying the valve timing. Their study revealed that instead of external EGR, residual exhaust gas due to negative valve overlap would slow down the heat release rate, decrease the pressure rise rate and the maximum combustion temperature, and reduce the NO_x emission simultaneously.

Yacine Rezgui [113] in his analytical work with ANSYS-CHEMKIN multi-zone model studied the effect of hydrogen addition to the primary reference fuel PRF-85 on its combustion characteristics in HCCI mode of operation. The results indicated that hydrogen dilution effect, irrespective of percentage of hydrogen, retarded combustion phasing, decreased both combustion duration and specific fuel consumption, and boosted the engine thermal efficiency.

Bharath and Tarek [114] stated that the performance and reliability of hydrogen fuelled homogeneous charge compression ignition (HCCI) engines are highly dependent on mixture formation methods. For preparing an ideal in-cylinder hydrogen-air mixture and control the auto-ignition process, the authors carried out computations with fuel injection strategies based on multiple-pulse direct injection (DI) as well as combinations of port fuel injection (PFI) and direct injection. They concluded that multiple DI and hybrid PFI/DI schemes could be used for varying load requirements that would lead to an extension of the operating range of HCCI engines. They observed a combination of volumetric auto-ignition and localized high-temperature burning.

Kozlov et al. [115] in their 2D CFD simulation study on HCCI engine with iso-octane fuel blends comprising hydrogen or syngas for two values of fuel-to-air equivalence ratio $\phi = 0.4$ and 0.2 . They observed for leaner mixture with $\phi = 0.2$ that addition of H₂ or syngas retarded the ignition and decreases the combustion duration. For $\phi = 0.2$ and $\phi = 0.4$, the increase of the specific indicated work was observed with addition of H₂ to iso-octane. The opposite tendency is detected when syngas H₂/CO = 2/1 is added to iso-octane. They observed higher emission indices of NO₂ and N₂O, compared to that of NO and concluded that N₂O, a more harmful gas,

should be considered as a part of evaluating the total emission of the engine at low load regimes.

Conclusion:

Hydrogen being a high energy carrier is a good choice for use in internal combustion engines as an alternative fuel due its excellent thermo-physical and combustion property. It can assist in improving the performance of engines when added to conventional fuels and helps to reduce NO_x, CO₂ and PM emissions. The concerns of backfire and cost of production and cost of storage has to be addressed for gaining full advantage from the use of hydrogen. Of late efforts underway to obtain hydrogen through bio-sources rather than steam reforming or electrolysis to make it more environmentally friendly.

HCCI mode of operation further helps in simultaneous reduction NO_x and PM emissions. HCCI concept throw open challenges with regards to homogeneous mixture formation, combustion phasing and high peak pressures with poor full load capabilities. Through 3D modelling and simulations, it has been proved that the use of swirl is beneficial to address the challenges being faced by the HCCI mode. However, HCCI engines still have unresolved issues, which are knocking and high levels of unburned HC and CO emissions. (The CO and HC emissions can be reduced with catalytic converter).

Since the combustion process is complex due to inter play many factors, numerical methods shows a great advantage over experiments to simulate the combustion behaviour in terms of cost and time and optimization can also be done with parameters affecting. It is established that hydrogen is best suited for making a homogeneous and lean mixture with air. Hydrogen as single fuel may not yield good results and even biofuels also but hydrogen addition will yield better.

Excess air ratio (λ) was observed to be a dominant factor in making HCCI operation feasible and obtaining lower NO_x emissions, much lower than with conventional engine operation. It is proved that negative valve overlap would be a better choice than external EGR to reduce NO_x emissions while slowing down the heat release rate, decrease the pressure rise rate and the maximum combustion temperature, and reduce the NO_x emission simultaneously. Hydrogen addition has helped in reduction of ignition delay time and overall it is concluded that partially fuelled HCCI mode is promising in terms of improving performance and reduction of emissions.

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