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Hydrogen and Natural Gas Comparison in Diesel HCCI Engines-A Review

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Abstract—**Homogeneous charge compression ignition (HCCI) enginesuse a new mode of combustion. The new challenges in developing HCCI engines arethe difficultiesin: controlling the auto-ignition of the mixture and the heat release rate at high load operation, achieving a cold start, meeting emission standards and controlling knock. At low engine speeds, early auto-ignition can occur, possibly leading to knocking, while late auto-ignition at high engine speeds will make HCCI susceptible to misfire. Hydrogengreatly reduces emission levels but with reduced power. However, when it is combined with diesel in dual fuel mode, low NO_x, CO and particulate matter emission levels are achieved while increasing engine efficiency by 13-16%. Numerical methods areused to predict HCCI engines' performance, which is cost efficient compared toexperimentation alone. The multi-zone method promises better simulation results by combining detailed chemical kineticswith simplified 3Dmodellingso that turbulence and inhomogeneity in the mixture are considered; good agreement between simulations and experiments has been achieved. Specific strategies used in the experimental and numerical methods, and other issues associated withHCCI engines are discussed in this paper.**

Keywords-component; HCCI; hydrogen; diesel; numerical

I. INTRODUCTION

Internal combustion (IC) engines have been widely used in numerous applications throughout the world. A new mode of combustion is being sought in order to reduce the emission levels from vehicles and one of the new modes is Homogeneous Charge Compression Ignition (HCCI) engines. HCCI is defined as the process by which a homogeneous mixture of air and fuel is compressed under such conditions that auto-ignition occurs near the end of the compression stroke, followed by the combustion process that is significantly faster than conventional diesel or Otto combustion[1]. It can provide high efficiency while maintaining low emissions and can be used in both modified spark ignition (SI) and compression ignition(CI) engines with any fuel or combination of fuels. The mixture in HCCI engines auto-ignites in multiple spots and is then burned volumetrically without discernable flame propagation[2,3].Combustion takes place when the homogeneous fuel mixture has reached the chemical activation energy and is fully controlled by chemical kinetics rather than spark or injection timing.

Since the mixture is lean and fully controlled by chemical kinetics, there is a new challenge in developing HCCI engines as it is difficult to control the auto-ignition of the mixture and the heat release rate at high load operation, achieve cold start, meet emission standards and control knock[4,5]. The advantages of HCCI engines are:1. the same or even better power band compared to SI or CI engines,2. high efficiency engines due to no throttling losses and high compression ratio, 3. ability to be used in any engine configuration: automobile engines, stationary engines, high load engines or small size engines. However, HCCI engines have their own disadvantages such as high level of unburned hydrocarbons (UHC) and CO [4,6,7]as well as knocking issues if the mixture is relatively inaccurate[4,6,8]. Emissions regulations are becoming more stringent and even though CO, $NO_x$and smoke emissions level in a HCCI enginehave been reduced while maintaining efficiencies close to those of diesel CI engines[6], knocking is still the major issue because of its sudden onset. Knocking is due to premature combustion where the ignition takes place before the piston reaches top dead centre (TDC) and it reduces enginereliability due to high vibration effects. The comparison analysis between natural gas and hydrogen is important as it will determine which fuel performs better with fewer issues.

This paper consists of five sections, where the next section will discuss the performance comparison between natural gas and hydrogen in HCCI mode. Section III presents the ignition control of HCCI engines, while the subsequent section will be on relevant numerical studies, followed by the conclusion.

II. PERFORMANCE COMPARISON

A. *State of the Art Current Internal Combustion Engines*

People are lookingfor ways to develop less polluting engines and some new technologiesare:

1. Turbo-Stratified Injection (TSI)
2. Fuel-Stratified Injection (FSI)
3. Homogeneous Charge Compression Ignition (HCCI)

TSI engines have been commercially used by Volkswagen for SI engines in which the vaporized fuel is directly injected into the combustion chamber at high pressure using multipoint injectors. This allows the fuel to mix homogeneously with air during the compression stroke. Furthermore, pressurized intake air will assist the combustion and therefore produce better efficiency,allowing small engines to be built with power and torque similar to bigger size engines.

FSI also uses direct injection fuel but uses a guideinside the intake manifold so the air enters the combustion chamber at a certain angle.With the help of the piston crown design, the air will experience swirl effects inside the chamber. This in turn will help the fuel mix with air homogeneously. It has been commercially used by Audi.

HCCI engines can be considered as newcomers even though the research was initially by Onishi*et al.* in 1979, as reportedin [9]. Investigators worldwide are developing HCCI engines as this technology has not matured sufficiently. They can be used in either SI or CI engine configurations with a high compression ratio (CR). HCCI engines work without the help of diesel injectors or spark plugs and can achieve high engine efficiency with low emission levels. General Motors Corporation (GM) has unveiled a prototype car with a gasoline HCCI engine and it was claimed that it could cut fuel consumption by 15%[10]. The engine is able to virtually eliminate NO_x emissions and lowers throttling losses which assists better fuel economy[11].

B. Fuels Used in HCCI Engines

HCCI engines can operate using any type of fuelas long as the fuel can be vaporized and mixed with air before ignition[12]. Since HCCI engines are fully controlled by chemical kinetics, it is important to look at the fuel's auto-ignition point to produce smooth engine operation. Different fuels will have different auto-ignition points and Fig.1shows the initial intake temperature required for the fuel to auto-ignite when operating in HCCI mode. It is clearly seen that methane requires a high intake temperature and high compression ratio to auto-ignite, as does natural gas because its main component (typically in a range of 75%-95%) is methane.

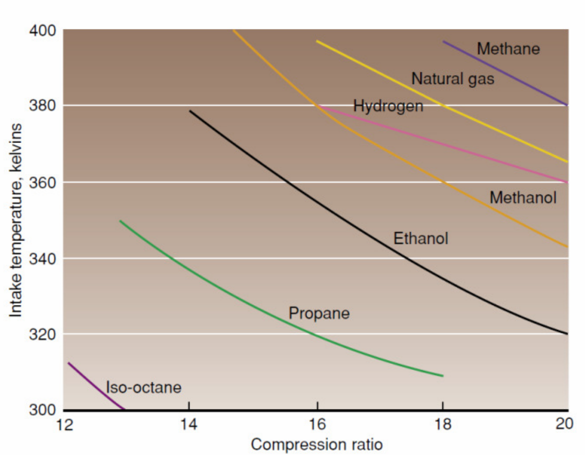

Figure 1. Intake temperature required for fuels to operate under HCCI mode with various compression ratios[12].

The component composition in natural gas varies for different countries as shown in Table I. It is easily adapted for use as a fuel due to its wide availability, economic and environmentalbenefits [13]. Its high auto-ignition point gives it a significant advantage over diesel-natural gas operation by maintaining the high CR of a diesel engine and lowering emissions at the same time[13-15]. It was found that methane is suitable for high CR engine operations[14] and results from a four stroke HCCI engine simulation have shown that methane did not ignite if the intake temperature was less than 400K with CR=15 [16]. This is supported by Fig. 1, where methane will only auto-ignite with intake temperature less than 400K when CR>18.

TABLE I. THE DIFFERENCE IN NATURAL GAS COMPOSITION BETWEEN SOME COUTRIES[2,3,13,17].

Components	**% Volume**			
	Australia	***Greece***	***Sweden***	***US***
Methane (CH_4)	90.0	98.0	87.58	91.1
Ethane (C_2H_6)	4.0	0.6	6.54	4.7
Propane (C_3H_8)	1.7	0.2	3.12	1.7
Butane (C_4H_{10})	0.4	0.2	1.04	1.4
Pentane (C_5H_{12})	0.11	0.1	0.17	-
Hexane (C_6H_{14})	0.08	-	0.02	-
Heptane (C_7H_{16})	0.01	-	-	-
Carbon Dioxide (CO_2)	2.7	0.1	0.31	0.5
Nitrogen (N_2)	1.0	0.8	1.22	0.6

If the Indicated Mean Effective Pressure (IMEP) is increased, it can reduce the intake temperature required on a HCCI engine. Increasing the CR has the same effect [17]. However, the intake temperature required for hydrogen is lower than that for natural gas in HCCI engines without increasing the IMEP or the CR [18]. This is due to hydrogen having a lower density than natural gas.Hydrogen can operate as a single fuel in a HCCI engine but it works in an unstable condition and is prone to generate knocking [19]. It has the highest diffusivity in air, about 3-8 times faster, which leads to fast mixing [15] andthe intake charge can be considered homogeneous when mixed with air[19]. Its net heating value is almost 3 times higher than diesel (119.93 MJ/kg compared to 42.5 MJ/kg) with a high self-ignition temperature to initiate combustion (858 K) [20].

Hydrogen and natural gas are mainly used as fuel additives or even as a single fuel in IC engines due to their practicality and availability. Car manufacturersare producing carspowered by fuel-cells(using hydrogen), as well as engines operated with compressed natural gas (CNG). They are purposely built to reduce emissions and be more economical than gasoline and diesel. Iso-octane is used as a surrogate fuel for gasoline in engine experiments while n-heptane is used for diesel[21]. Alcohol-derived fuels, as shown in Fig. 1, are not widely used due to their complexity to produce.

C. Natural Gas and Hydrogen Operating Conditions

Natural gas or hydrogen, when combined with diesel in combustion, yield low emissions and to some extent increase the engine efficiency, either in HCCI or CI combustion modes.

Diesel alone is not suitable for HCCI engines due to its low volatility and high propensity to auto-ignite, while natural gas has a high resistance to auto-ignition[22]. Combinations of high octane number fuels (natural gas) with high cetane number fuels (diesel) help in stabilizing the combustion in dual fuel mode where diesel is used as an ignition source[19,23]. Hydrogen on the other hand has a high octane number as well as high net heating value and combination with diesel helps in increasing engine efficiency and controlling the auto-ignition point in HCCI engines. Table IIcompares the chemical properties of diesel with natural gas and hydrogen.

TABLE II. DIESEL PROPERTIES COMPARED TO HYDROGEN AND NATURAL GAS[15,20,24,25]

Properties	Diesel	Hydrogen	Natural Gas
Main component	-	-	Methane (CH_4)
Auto-ignition Temperature (K)	553	858	923
Lower heating value (MJ/kg)	42.5	119.93	50
Density (kg/m^3)	833-881	0.08	692
Molecular weight (g/mol)	170	2.016	16.043
Flammability limits in air (vol%)	0.7-5	4-75	5-15
Flame velocity (m/s)	0.3	2.65-3.25	0.45
Specific gravity	0.83	0.091	0.55
Boiling point (K)	453-653	20.2	111.5
Cetane number	40-60	-	-
Octane number	30	130	120
CO2 emissions (%)	13.4	0	9.5
Mass diffusivity in air (cm^2/s)	-	0.61	0.16
Min ignition energy (mJ)	-	0.02	0.28

Hydrogen has the largest lower heating value (LHV) or net calorific value compared to both diesel and natural gas, which means it releases a high amount of energy during combustion and thus produces the highest flame velocity. The wide range of the flammability limits allows a wide range of engine power outputs through changes in the mixture equivalence ratio. The flammable mixtures of hydrogen can go from as lean as $\lambda = 10$ to as rich as $\lambda = 0.14$[25], where λ is the air to fuel equivalence ratio.

D. *Brake Thermal Efficiency*

The brake thermal efficiency (BTE) of an engine is the ratio of brake power output to power input and describes the power produced by an engine with respect to the energy supplied by the fuel. Biogas is produced by the anaerobic fermentation of cellulose biomass materials [14] and its main component is methane (>70%). A test has been performed using biogas on energy ratio ranges from 40% to 57% and intake temperatures of 80°C, 100°C and 135°C [6]. It was found that the best combination of energy ratio with diesel in HCCI mode was 51% biogas and the optimum efficiency occurredwhen the intake temperature was 135°C. High energy ratios lower the heat release rate and the efficiency [6]. However, even when operated at the optimum biogas energy ratio, the BTE was no better than diesel running in CI mode.Duc and Wattanavichien[14] also worked on dual fuel biogas-diesel operating in non-HCCI mode at full load. The diesel substitution was about 36% at the lowest engine speed. They reported that biogas-diesel running in dual fuel mode has a lower efficiency than diesel as a single fuelin either HCCI or non-HCCI mode.

Hydrogen on the other hand had a higherBTEthanpure dieselin non-HCCI mode, increasing the BTE up to 13-16% [15]. Szwaja and Grab-Rogalinski[19] found that the BTE was increased from 30.3% to 32% with 5% hydrogen addition. The increase of BTE in hydrogen-diesel mode might be due to the uniformity of mixing of hydrogen with air[20]. Hydrogen as a single fuel running in HCCI mode gives BTE up to 45%[18], showing that hydrogen is able to operate with extremely lean mixtures and still maintain a relatively high efficiency compared to diesel engines. Table III shows that hydrogen in HCCI mode yields better resultscompared to conventional mode (45% vs 42.8%) and hydrogen with diesel in non-HCCI mode produces higher efficiency than diesel alone [26]. This conclusion was also reached when reformed exhaust gas recirculation (REGR) was used with hydrogen-rich gas (no more than 24%) added to the intake manifold [27].

TABLE III. MAXIMUM BTE FOR HYDROGEN-DIESEL FUEL[26,27]

	Diesel DI	Dual fuel (H_2+diesel)	H_2+Diesel PPCCI	H2 HCCI	H2 DI
BTE (%)	27.9	33.9	36.5	45.0	42.8

E. *Peak Pressure and Temperature*

The variations of heat release rate during combustion affect the in-cylinder peak pressure and temperature. All these quantities depend on the speed of the engine, equivalence ratio, load, intake pressure, temperature and energy content of the fuel configurations. Higher loadsand richer mixtures typically produce higher peak pressures. Table IV shows howthe in-cylinder peak pressure and temperature vary for HCCI and conventional CI modes. These are general data to illustrate which mode produces higher peak pressure. The data for temperature is incomplete but in general, temperature increases with pressure.HCCI configurations produce lower peak pressure than conventional CI modes for every fuel configuration, leading to significant impacts on emission levels. It can be concluded that the hydrogen fuel configuration yields the highest peak pressure and therefore produces better power and efficiency. Hydrogen addition to diesel influences the peak pressure generation. The higher the addition, the higher the peak pressure is, andthe addition of hydrogen is able to reduce ignition delay as well [19].

F. *Emission Levels*

Emissions in HCCI engines consist of UHC, CO, NO_x, soot and particulate matters. UHC and CO emissions in HCCI engines arereported by most researchers to be higher than conventional diesel engines. This might be due to incomplete combustion caused by low combustion temperatures [7,28], which cause deposition of fuel in boundary layers and crevices[29]. Results of simulations confirm that thepiston-ring crevice needs to be resolved in order to predict UHC and CO emissions[4]. UHC and COemissions originate in the crevices and boundary layer, which are too cold for complete consumption [30].However, the difference in NO_x emission levels between natural gas and hydrogen in diesel HCCI mode might be due to different causes. In biogas-diesel HCCI engines,the NO_x level is low when the biogas energy was increased[6]. Olsson *et al.*[17] stated thatNO_x level is low in natural gas HCCI engines and when combined with exhaust gas recirculation (EGR), it goes down further[7]. Even in natural gas-diesel non-HCCI mode, the NO_x level is lowerthan diesel conventional CI engines [31].Hydrogen on the other hand produces zero UHC, CO and CO2, due to the absence of carbon in the fuel, but still producesNO_x[25]. Hydrogen operated as a single fuel in CI mode yields lower NO_x levelsthan diesel[26]. When it is combined with diesel and operated in non-HCCI mode, lower NO_x emissions are obtained for all load ranges compared to diesel in conventional mode[15]. They reported that the formation of NO depends on temperature more than the availability of oxygen. Therefore, the hydrogen-diesel in HCCI mode results in extremely low NO_x emissions level with no significant amount of smoke[32].

TABLE IV. IN-CYLINDER PEAK PRESSURE AND TEMPERATURE COMPARISON FOR NATURAL GAS AND HYDROGEN IN VARIOUS CONFIGURATIONS[6,18,26,29,33,34]

Mode	Max Pressure (MPa)		Max Temperature (K)	
	HCCI	*CI*	*HCCI*	*CI*
H_2	~ 8	~ 12	-	-
NG	~ 7	~ 7.5	~ 1300	~ 1850
Diesel	~ 6.1	~ 6.6	-	~ 2300
NG + Diesel	~ 3	~ 5.5	~ 1450	-
H_2 + Diesel	~ 7	~ 7.8	-	-

TABLE V BMEP RANGE FOR VARIOUS ENGINES TYPES[36]

Engine Type	Compression Ratio	BMEP Range (MPa)
SI Engines		
Small (Motorcylces)	6-11	0.4-1
Passenger cars	8-10	0.7-1
Trucks	7-9	0.65-0.7
Large gas engines	8-12	0.68-1.2
Diesel Engines		
Passenger cars	17-23	0.5-0.75
Trucks	16-22	0.6-0.9
Large trucks	14-20	1.2-1.8
Locomotive	12-18	0.7-2.3
Marine engines	10-12	0.9-1.7

G. BMEP

The brake mean effective pressure (BMEP)is an effective comparison tool to measure engine performance and indicates an engine’s capacity to produce power output over the full engine speed range. It is also used to compare one engine’s performance with another. A high BMEP shows the ability of the engine to perform high load operations. One of the HCCI engine’s challenges is limited load range where high load operations of HCCI engines tend to produce knock [22]. Table V shows the BMEP ranges of standard engines.

Natural gas-diesel in HCCI mode operates in the BMEP range of 0.25 – 0.4 MPa[6], which is low compared with the engines in Table V. To increase the BMEP,the concentration of natural gas should be increased but this will lead to knocking if a high amount of natural gas is used with diesel. Fig. 2 shows the best energy ratio for natural gas-diesel HCCI mode is about 51% and within the circled range. In this optimized energy ratio, the maximum BMEP is only 0.4 MPa. This is a very limited load range and is not suitable for high load engine operations.

Hydrogen with diesel in HCCI mode on the other hand shows that the engine operation is stable up to 0.6 MPa BMEP[27,32]. If a supercharger isused in hydrogen-diesel dual-fuel mode on a non-HCCI engine, a maximum BMEP of 0.91MPa was reported[35]. Therefore, hydrogen and diesel in HCCI mode might be able to be used for high load engine operations.

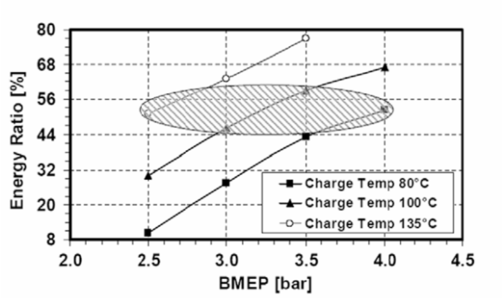

Figure 2. Best energy ratio for natural gas-diesel HCCI engines[6].

H. Knocking

Knocking is physically detected when the engine vibrates too much and apinging sound can be heard outside as a result of the combustion activity. If not controlled, knocking could lead to severe engine damage and shorten its life. Knocking can happen in any reciprocating engine. HCCI engines are prone to knock since they are controlled by chemical kinetics and there is no fixed mechanism to control knock in them. Knocking issueslimit the load range of a HCCI engine: high load operations can easily initiate knock, soupper load limits have to be applied[7]. Knocking and misfire are two different behaviors which must be avoided in engine operation as both of them deteriorate engine performance.In natural gas-diesel HCCI engines, a misfire occurs when a high natural gas flow rate is combined with a low diesel flow rate while knocking starts withthe opposite configuration [6]. If HCCI engines operate on hydrogen-diesel fuels, knocking will easily occur depending on the amount of hydrogen added. If the HCCI engine runs on natural gas with dimethyl ether(DME), the knock limit is at an in-cylinder pressure of 9 MPa and a very limited load range is obtained while getting unstable operation for high natural gas concentrations. This was discovered by using Computational Fluid Dynamics (CFD) simulations with detailed chemical kinetics [22]. An investigation of auto-ignition and combustion of natural gas HCCI engines showed that knocking starts to happen when the equivalence ratio is more than 0.45 with an intake temperature of 380K[8]. Fig.3 shows the area of knocking and misfiring of natural gas HCCI engines with constant intake pressure. Thus, natural gas HCCI engines will not be able to operate at high load conditions due to this limitation.

Knock occurs when a rapid release of energy in the remaining unburned mixture causesa rapid increase in local pressures. In hydrogen-diesel engines, knocking will take place when the fraction of total energy contained in hydrogen is more than 16% [19]and the engine will not work in a stable condition if 100% hydrogen is used. A combination of hydrogen and diethyl ether (DEE) produced severe knock on 100% load[20]and higher hydrogen content leads to a higherprobability of knock onset. Knocking phenomena can be traced from the in-cylinder pressure variations, observing the instantaneous local pressure rise. The graph formed depends on the knocking frequency: the higher the frequency, the more severe the knock [19].However, there is no concrete mechanism in the literature describing the knocking phenomenon in HCCI engines and the methods to control it. In SI engines, it is quite easy to control knock: car manufacturers usually install knock and oxygen sensors in the engine. If the mixture is prone to generate knock, they will adjust the spark timing accordingly. But in HCCI engines, there is no spark to control such situations andit all heavily depends on the right mixtures and conditions.

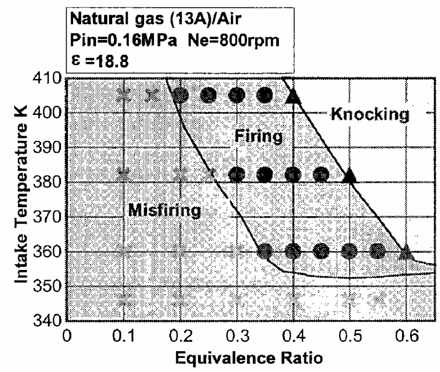

Figure 3. Knocking and misfiring area for natural gas HCCI engines under constant intake pressure [8]

III. Ignition Control In HCCI Engines

Ignition control is one of the challenges in HCCI enginesandthe challenge includes auto-ignition control, limiting the heat release rate at high load operations and meeting emissions standards while providing smooth engine operation, achieving cold starts or startability of the engine and limited load range [5,30]. A study of ignition control of HCCI engines has suggested that ignition can be controlled by using promoters or additives, blending of low cetane number fuels with high cetane number fuels[37],pre-heating of the intake air, pressurizing the intake air, hydrogen addition and varying the amount of exhaust gas recirculation (EGR) through early closure of the exhaust valve.

A. Pre-Heat Intake Air

Some fuels which are operated in HCCI modesuch as methane, natural gas and hydrogen, require a high intake temperature. By pre-heating the intake air, ignition delay is reduced and thus the ignition timing can be controlled. As shown before, methane and natural gas require high temperatures to auto-ignite and methane did not ignite for an intake temperature of 400K[37]. Therefore, it is imperative to pre-heat the intake air to make the fuels combust smoothly.Questions may arise from this implication whether it is practical to include electric heaters [8] in an engine bay just for this purpose. The heater causes the operation and maintenance costs to increase and contributes to extra engine weight. Installing a heater is an option used by most researchers as the easiest way to get intake air heated to some specific temperature.

B. Pressurized Intake Air

Turbochargersand superchargers are commonly used in real engine applicationsbecause they can be applied toany internal combustion engine. The operational concepts of these two chargers are the same: to provide a high intake pressure into the combustion chamber and thus increase the engine performance. Some studies show that the start of combustion (SOC) is advanced if the intake pressure is increased by 0.1 MPa. This indicates that pressurized intake air is able to improve the auto-ignition of the fuel [38]. However, these situations also depend on the type of fuel used, and in this case they used primary reference fuels and gasoline. By increasing the intake pressure, they managed to get the auto-ignition to start at 15° before top dead center(BTDC).On the other hand, supercharging (pressurizing intake air) is able to increase engine efficiency [5]. A supercharged hydrogen-diesel engine, but in non-HCCI mode, was able to maintain high thermal efficiencies and it was possible to use more than 90% hydrogen energy substitution for the diesel[27].

C. Hydrogen Addition

Hydrogen addition to the HCCI engine is one of the effective waysto control the ignition timing since hydrogen is able to reduce ignition delay time effectively. Furthermore, hydrogen can be produced from the exhaust gases of the engine itself using a reformer, which is called an“on-board hydrogen producer” [7,32]. As the amount of hydrogen was increased, auto-ignition delay time reduced accordingly while the in-cylinder peak pressure increased, ignition temperature reduced and indicated power increased [1]. The use of hydrogen addition does not involve high cost since it uses a lower-pressure fuel-injection system[30]. Hydrogen addition to a diesel engine will retard the heat release rate and delays the temperature rise. Furthermore, the addition of hydrogen is able to increase the engine efficiency by a significant margin[15,20]. By using a catalytic reforming aid in HCCI,the addition of hydrogen in natural gas HCCI engines helps in decreasing the need for high intake temperatures and also is a means of extending the lower limit of HCCI operations[39].

D. Exhaust Gas Recirculation (EGR)

EGR is used to reducethe large heat difference between peak pressure and intake pressure. This means that the intake temperature of using EGR is high and certainly helps in auto-ignition of the mixtures. Besides increasing the BTE of the engine, EGR is able to reduce NO_x formation as well[15]. Furthermore, EGR improved auto-ignition of the engine and reduced the in-cylinder peak pressure. EGR used in a diesel HCCI engine showed an improvement of 1.1% engine efficiency, advanced the auto-ignition by 10° and reduced the heat release rate by 11 J/° CA compared to diesel fuel[28]. Ganesh and Nagarajan[40]found that by using EGR on diesel HCCI engines they were able to reduce heat release by absorbing heat during combustion. They could control ignition delay as well as reduce combustion temperature and pressure. However, using EGR leads to a power loss of 20% compared to diesel fuels[29].

IV. Numerical Study Of HCCI Engines

Simulations are used to reduce research costs while maintaining good productivity because of its cost efficiency compared to solely experimentation. By using numerical methods, one can optimize engine parameters before doing experimentsand get optimized parameters within a short time and low cost. Most researchersuse KIVA-3V CFD software in combination with detailed chemical kinetics solutions using CHEMKIN from Sandia National Laboratories[41-45]. Good agreement between simulations and experiments has been achieved, however it depends on the numerical methods used.

A. Numerical and CFD Environments

Numerical modeling can be categorized by the number of dimensions considered: zero-dimensional, quasi-dimensional and multi-dimensional. CFD is a multi-dimensionalmethod whereby it resolves very small-scale zones and typically produces a more accurate result. A zero-dimensional model is the simplest model where there is only one independent variable, typically either time or, equivalently, crank angle,and uses an empirical heat release model. However, the disadvantage of this method is that the simulated combustion duration is shorter than the actual duration due toinhomogeneities in reality [9]. The calculation results of zero-dimensional models produce rapid pressure increases and very high heat release rates compared to actual HCCI enginecombustion[46]. A quasi-dimensional model uses a turbulent sub-model for turbulent combustion and to derive a heat release model.Fig. 4 shows three different interacting zones in a quasi-dimensional model. It is typically used to improve upon the zero-dimensional model. However, UHC emissions are over-predicted by 5-15% and CO emissions exhibit a 50% error. This is due to the inability of the model to capture small temperature differences in the crevices [47,48].

B. Single and Multi-Zone Models

A single-zone model is where the combustion chamber area is treated as one homogeneous block. Amulti-zone model separatesthe combustion chamber into several zones and the zone distribution depends on the type of the engine, either depending upon flame propagation or homogeneous mixtures. Multi-zone models can represent the inhomogeneity in the cylinder prior to combustion [9]. Fig. 5(a) shows the multi-zone model in HCCI engines while Fig. 5(b) is a three zone model of SI engines. Multi-zone modeling of HCCI enginesis organized in such a way because the heat generated in a HCCI engine comes from the core of the combustion chamber. This is different to SI engines where the zone is started from the spark plug, the location of the heat source, and propagated according to the flame front motion.

The single zone model has some limitations due to the assumption that the whole combustion chamber is treated as homogeneous. Peak cylinder pressure and rate of pressure rise can be over-predicted and the model cannot accurately predict CO and HC emissions, which primarily depend on crevices [37]. It predicts a very short burn duration and a very high peak cylinder pressure while the multi-zone model predicts the pressure trace and the peak cylinder pressurevery well. It also cannot consider boundary layer effect and crevices and thus cannot predict CO and HC emissions[51]. Fig. 6 shows the difference between single and multi-zone models, where the multi-zone model's results are close to the experiment. Adding a turbulent mixing model to the multi-zone model yields a better result than just adding a chemical kinetics model.

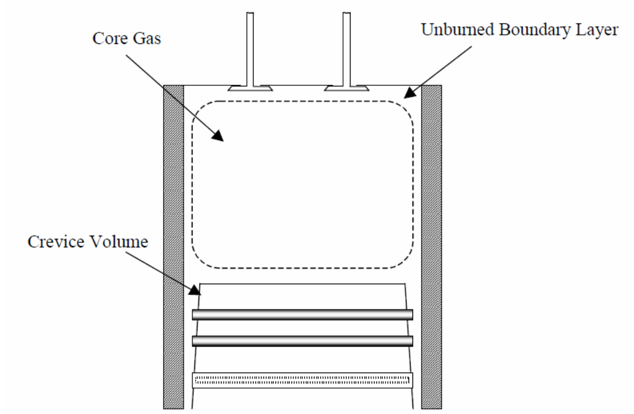

Figure 4. General layout of the quasi-dimensional simulation showing the interacting adiabatic core, thermal boundary layer and crevice regions [48].

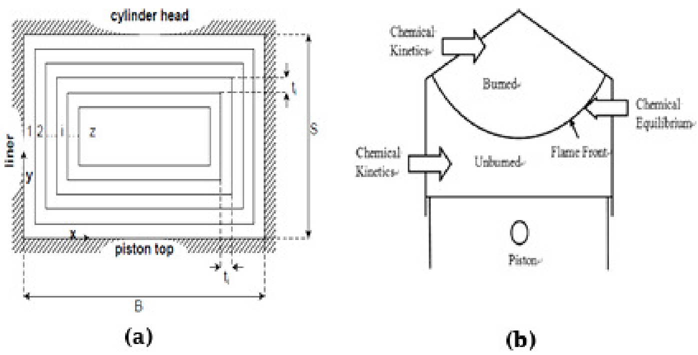

Figure 5. Multi-zone model geometric configuration difference (a) HCCI engine [49] (b) SI engines [50].

If there is any inhomogeneity in the mixture, turbulence has an effect on combustion.Better agreement in combustion phasing is achieved when using the multi-zone method coupled with detailed chemical kinetics and turbulent mixing effects [3]. The ignition timing was predicted correctly without the need to modify any constants. If the mixture is completely homogeneous, turbulent mixing has no or little effect on the combustion heat release rate. However, it is suspected that there will be inhomogeneities in the mixture as there is insufficient time to mix down to the smallest relevant scales possibly causing turbulent mixing to directly affect reaction rates[3,4]. In actual combustion chambers, transportation of chemical species, heat transfer and heterogeneity of temperature and species concentration exist[39]. Amulti-zone model of HCCI combustion predicts maximum pressure, burn duration, indicated efficiency and combustion efficiency with the worst error 10%. However, UHC and CO emissions are under-predicted;Aceves*et al.*[51]suggested that this might be due to some crevices not being considered in the analysis. They used a multi-zone model including zones in crevice regions with more accurate results.

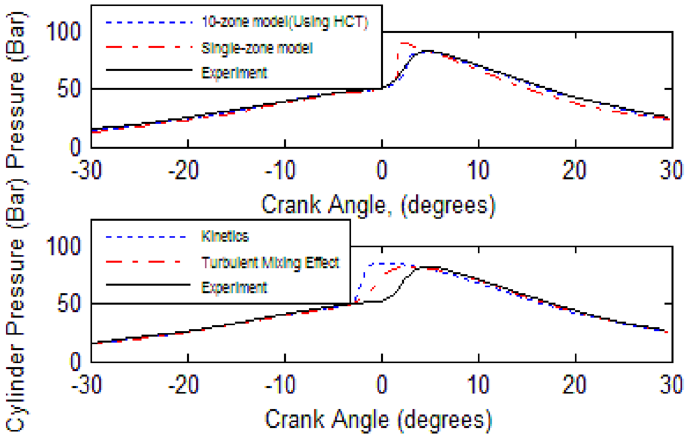

Figure 6. Comparison between single and multi-zone model [51].

C. *Multi-Dimensional Models: CFD*

A multi-dimensional model solves the equations for mass, momentum, energy and species conservation to get more accurate results at the expense of computational time and resources. When solving detailed chemical kinetics,a sequential operation is used to reduce computational time by solving the flow field then the chemistry rather than attempting to satisfy both simultaneously. Two common approachesto multi-dimensional modeling are multi-zone models and CFD. A multi-zone model requires substantially less computational time and resources than CFD at the expense of accuracy. However, Aceves*et al.*[52] showed that a 40-zone model can successfully predict the effect of crevice geometry on HCCI combustion with combustion efficiency predicted within 5% error compared to experiment.

A study has been performedusing two-step processes in CFD to analyze combustion[12]. First, KIVA CFD was used for the effect of turbulence to solve the transport of all variables. Then the result from KIVA was used in the hydrodynamics, chemistry and transport (HCT) code to calculate the combustion parameters. This two-step method made it possible to obtain accurate predictions for turbulent combustion within a reasonable computational time[12]. The effects of gas exchange processeson HCCI engine using the CFD methodshows that the proposed approach can provide an accurate prediction of the combustion process. The present modeling can account for mixture inhomogeneities in both temperature and composition [53].

D. *Turbulent Combustion Modelling*

Turbulent combustion modelsare used to predict the mixing process due to turbulence. Numerous models have been devised and validated against Direct Numerical Simulations (DNS) or experiments. A study of the turbulent-chemistry interactions during the ignition of a temperature-stratified mixture for HCCI engine modeling has been discussed [54]. They reported that the Euclidean Minimal Spanning Tree (EMST) mixing model[55] performed better than the other mixing models, where the new Multiple Mapping Conditioning (MMC) method [56] was not included. An investigation ofMMC has reported that the model is capable of predicting the mean temperature rise with reasonable fidelity and follows the stoichiometric temperature history better than the other models [57], as shown in Fig. 7.

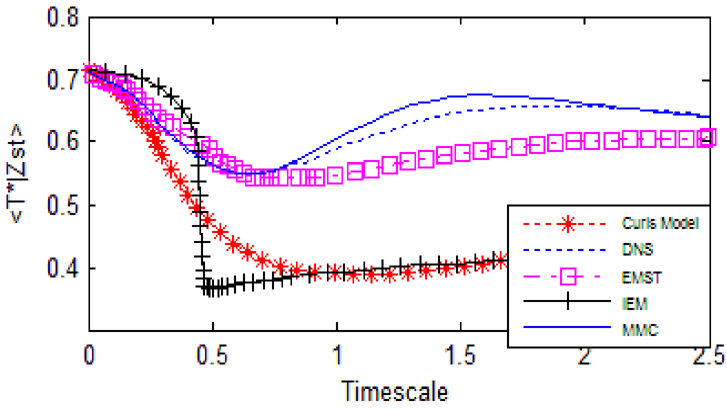

Figure 7. Stoichiometric temperature results for various mixing models [57,58]

V. CONCLUSION

It is clearly seen that the hydrogen-diesel combination shows better results for most major quantities compared to natural gas-diesel. It produces a higher efficiency compared to single diesel mode, low NO_x, CO, soot and particulate emissions. However, HCCI engines still have unresolved issues, which are knocking and high levels of HC and CO emissions. Further studies have to be performed in order to solve these remaining issues. To achieve this, the multi-zone numerical method shows promising results. This modeling technique, when combined with advanced turbulent mixing models, has the potential of producing good predictions of actual engines.

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