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Effects of Engine Parameters and Fuel Compositions on Ignition Timing and Emission Characteristics of HCCI Engine

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Abstract**—**In this research, the effects of the engine parameters like compression ratios and steam injection on igniting timing and emission characteristics have been investigated numerically. The in-cylinder temperature and pressure at four different compression ratios have been compared with numerical results, and they show a good agreement with the published data. Two different fuels have been used in this study: Isooctane (IC_8H_{18}), and ethanol (C_2H_5OH). The increasing of the compression ratio (CR) advances the ignition timing, decreases the burn duration and increases the temperature and the pressure. The injection of water vapor lower than 40% decreased the peak temperature and slowed the combustion rate which leads to a lower NOx emission.

Keywords**—**Compression ratio, emission, HCCI engine, ignition timing, steam injection.

I. Introduction

NOWADAYS, with the crisis of energy resources depletion and environmental pollution, research on the development of alternative combustion strategies drew the attention of the engineers. An alternative combustion technology, commonly known as homogeneous charge compression ignition (HCCI), has emerged, and it has the potential to decrease emissions and to achieve high efficiencies [1], [2]. The HCCI engine concept is a promising idea that combines the best of the spark-ignition (SI) and compression ignition (CI) engine. The SI engine is characterized by a homogeneous mixture of fuel and air before combustion initiation. Then, the charge is compressed and ignited by a spark plug. But, in the CI engine, the air is compressed to a higher pressure and the fuel is injected into the hot compressed air then the auto-ignition will be occurring. HCCI engines are working using a homogeneous mixture of the SI and compress this to auto-ignition like the CI [3].

Many fuels have been used to support the energy needs of the automobile and other combustion devices. In this work, we will focus on two different fuels: isooctane (IC_8H_{18}), and ethanol (C_2H_5OH). Iso-octane is a clean fuel, which contains a high octane number and not includes any aromatics, metals or sulphur. The ecological fuel (ethanol C_2H_5OH) has been used extensively as an additive or an alternative fuel in SIengines as well as in diesel engines, because it has a high-octane, clean-burning fuel [4], [5]. Furthermore, researcher [6]-[9] have been investigating in the field of the effect of CR in controlling the HCCI engines. CR is defined as the ratio of the maximum volume formed in the cylinder to the minimum volume (clearance volume). However, the study of CRs'effect is limited due to the difficulty of implementing a CR variation in an engine, either indirectly by variable valve timing [6], or directly by varying the cylinder volume. Machrafi et al. and Terashima et al. [7], [8] observed that an increase in the CR decreases the ignition delay. In 2013, an experimental study was conducted on single cylinder variable compression diesel engine with different CRsto estimate combustion and emission characteristics of the engine. It was found that the combustion duration was decreased by 2-3° with an increase in CR due to less ignition delay [9].

Another method controlling pollutants emissions is the use of steam injection. Kökkülünket al. [10] and Gonca [11] developed an Electronic Controlled Steam Injection (ESI) system, and they observed that NOx emissions decrease up to 33%. Murthy et al. [12] developed the solar generated steam injection to the diesel engine, and they conclude that NO emissions and exhaust temperature reduce; soot emissions, thermal efficiency, power and SFC increase at full load conditions.

The objective of this work is to predict the effect of CRsand Steam Injection on igniting timing and emission characteristics. The investigation range of the parameters is a Steam Injection between 0% and 80% (in steps of 20 %) and a CR between 13 and 19. The fuels that are used for this study are isooctane and ethanol, and their kinetic mechanisms are constructed by [13], [14], respectively.

II. Materials and Methods

A. Overview of Simulation Software

CHEMKIN [15] is a powerful set of software tools for solving complex chemical kinetics problems. It is used to study reacting flows, such as those found in combustion, catalysis, chemical vapor deposition, and plasma etching. CHEMKIN consists of rigorous gas-phase and gas-surface chemical kinetics in a variety of reactor models that can be used to represent the specific set of systems of interest (Fig. 1). An internal combustion engine (ICE) model has been used

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in this study to simulate the engine combustion behavior (Fig. 2).

The ICE module of the software is given by:

$$\frac{d(\frac{V(\theta)}{Vc})}{dt} = \Omega\left(\frac{\text{CR -1}}{2}\right)\sin\theta\left[\frac{1+\cos\theta}{\sqrt{\text{R}^2-\sin^2\theta}}\right] \quad (1)$$

where $V_{(\theta)}$: total volume available for combustion in the cylinder; θ is the crank angle; Ω, the rotation rate of the crank arm is given by:

$$\Omega = \frac{d\theta}{dt}$$

CR: compression ratio; *Vc*: clearance volume; R: the ratio of connecting the rod to the crank-arm radius.

B. General Input Parameters

The heat transfer correlation coefficients (a, b, and c) and Woschni Correlation coefficients (C11, C12, and C2) were the additional parameter to be defined to run the software. Theses coefficients were taken from [16], Tables I and II.

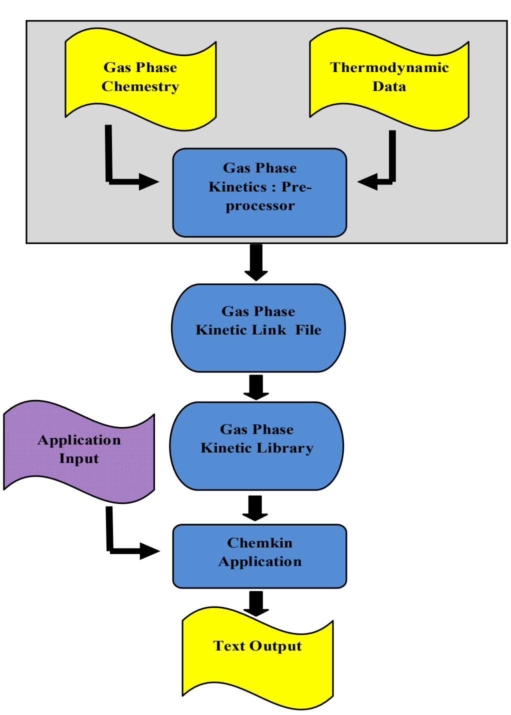


Fig. 1 Chemkin package working flow diagram [15]

TABLE I
HEAT TRANSFER CORRELATION COEFFICIENTS [16]

Coefficient	Values
a	0.035
b	0.071
c	0.0

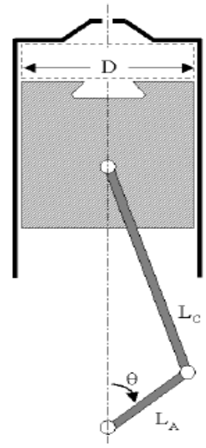


Fig. 2 Schematic view of an engine cylinder: L_A the connecting rod length; L_C: the crank arm radius. *D*: the bore diameter; θ is the crank angle [13]

TABLE II
THE WOSCHNI CORRELATION COEFFICIENTS [16]

Coefficient	Values
C11	2.28
C12	0.308
C2	0.324

III. RESULTS AND DISCUSSION

A. Fuel and Mechanism

Two different fuels have been used in the present investigation i.e. isooctane (C_8H_{18}), and ethanol (C_2H_5OH). Table III gives some basic properties of these fuels.

TABLE III
SELECTED FUEL PROPERTIES (AT 20° C AND 1 ATM)

Fuel	Chemical Formula	Molecular Weight (g/mol)	Octane Number
Isooctane	C_8H_{18}	114	100
Ethanol	C_2H_5OH	46	106

The model describing the isooctane oxidation is generated by [13]. The chemical kinetic mechanism is performed using 857 species and 3606 reactions. The study of the oxidation of ethanol is based on a detailed mechanism with 383 reversible reactions and 56 species, proposed by [14]. The engine specification used for this work is shown in Table IV.

TABLE IV
GEOMETRY OF ENGINE AND FIXED ENGINE OPERATING PARAMETERS

Parameters	Setting
Displaced Volume	587.622 cm3
Bore×stroke	72mm×120.6 mm
Ratio of the Connecting Rod length to crank Radius	3.59
Intake temperature (K)	430
Wall temperature (K)	415
Equivalence ratio	0.6-1
Engine Speed (rpm)	1000.0
CR	13–24
Fuel	Isooctane or Ethanol

B. Validation

The predicted in-cylinder temperature and pressure are plotted in Figs. 3 and 4, respectively. Those figures demonstrate that our numerical results show a good agreement with Rahbari's [17] results. In our study, computations were performed using the CHEMKIN computer code. It is able to simulate the HCCI engine for the combustion process at all the operation parameters.

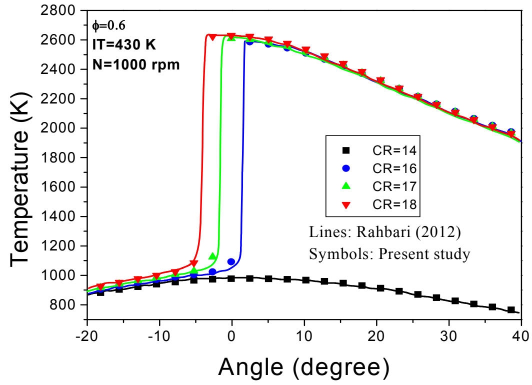


Fig. 3 Variation of temperature versus crank angle for different CR Comparison of our numerical result with Rahbariresult [17]

C. Fuel Composition

1.Effect on Ignition Timing

Ignition delay is the period between the beginning of fuel injection into the combustion chamber and the start of combustion. The CR effect in a lean mixture ($\varphi = 0.6$) is presented in Figs. 5 and 6, using ethanol or isooctane as a fuel. For ethanol, the combustion process does not occur if the CR is lower than 14. However, by using isooctane as a fuel; the combustion process does not occur if the CR lowers than 13. These results can explain by the effect of the octane numbers: fuels with lower octane numbers (isooctane) are ignited more easily. The octane number gives the standard measure of the engine performance. As a result, fuel with a higher octane number can provide more compression and then an efficient combustion.

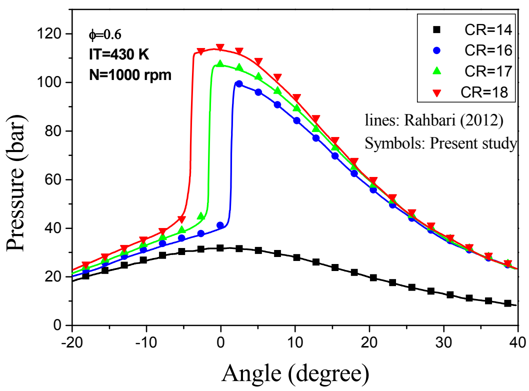


Fig. 4 Variation of pressure versus crank angle for different CR Comparison of our numerical result with Rahbari result [17]

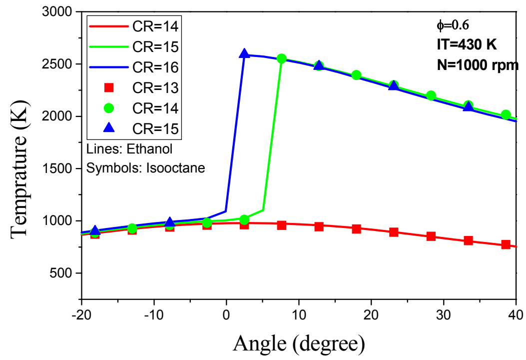


Fig. 5 Effect of CR, from 13 to 16, on HCCI: Comparison between two different fuels

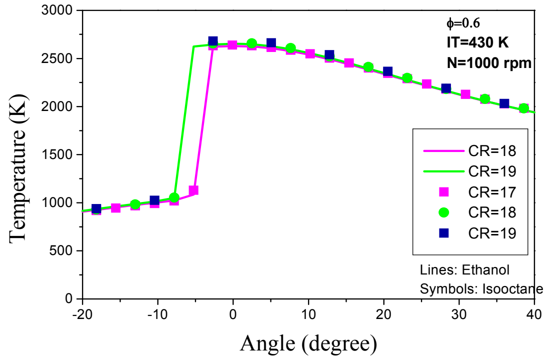


Fig. 6 Effect of CR, from 17 to 19, on HCCI: Comparison between two different fuels

2.Engine Emission Studies

Emission of different exhaust gas species (CO2, and CO) is presented in this section. The pollutant emissions resulting of the combustion of isooctane (or ethanol) with air are presented in Fig. 7. It reveals that CO and CO_2 productions yield similar values for isooctane and ethanol. It is also observed that isooctane combustion generates less H_2O than the comparable levels ethanol. The presence of oxygen in the chemical composition of the ethanol as a fuel will generally contribute to larger levels of species composed of oxygen in rich conditions than non-oxygenated fuels.

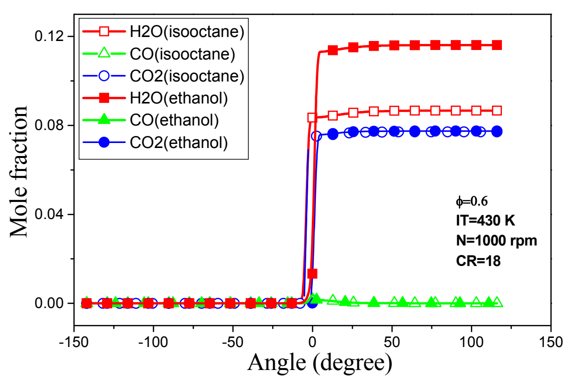
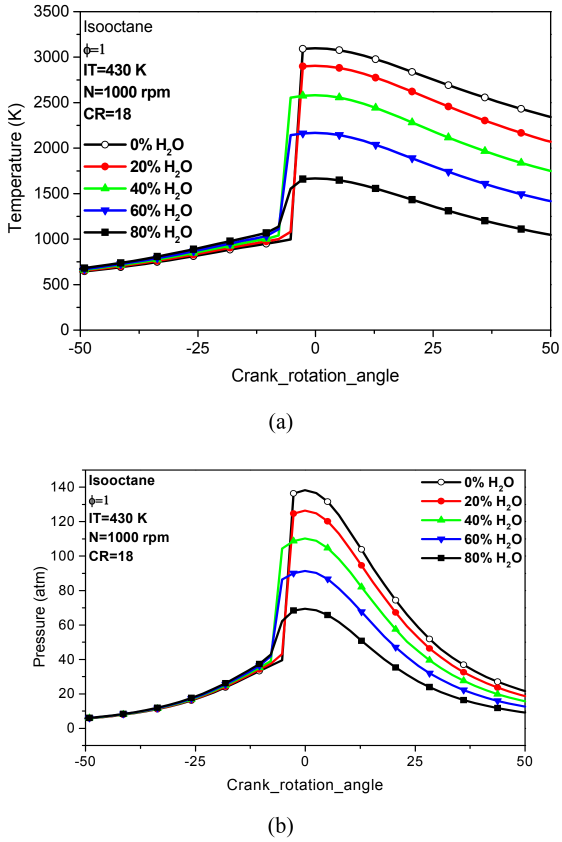


Fig. 7 Pollutants Emissions Profiles from the Combustion of two Fuels



(a)

(b)

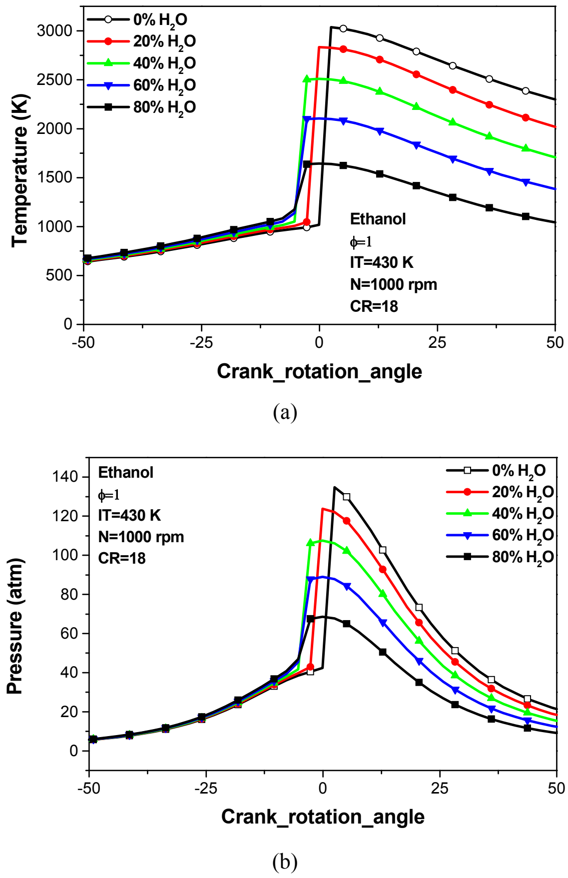
Fig. 8 (a) Mean temperature variation with steam injection ratio using isooctane as a fuel (b) Mean pressure variation with steam injection ratio using isooctane as a fuel

D. Steam Injection

1.Effects on Ignition Timing

Figs. 8 (a) and (b) present respectively the variation of the mean temperature and pressure with steam injection, of HCCI engine operation, fueled with isooctane. Those results are obtained with a CR equal to 18, in a stoichiometric mixture. The intake temperature is fixed to 430 K. In this part of the work, the steam injection varied from 0% to 80% with a step of 20%. The injection of the vapor in the mixture reduce the NOx emissions the by increasing the peak temperature. However, it has a negative effect on engine performance by decreasing the peak pressure. For diesel engine, it is not recommended to reduce the maximum pressure more than 20% [7].

Using the ethanol as a fuel, the variation of the temperature and pressure with steam injection, are presented in Figs. 9 (a) and (b) respectively. Fig. 9 (a) shows that the injection of steam reduced the peak temperatures and then reducing NOx emissions. Injection of water vapor in the ethanol (20% H_2O; 40% H_2O; 60% and 80% H_2O) decreases the temperature, the combustion speed, and the peak pressure. According to the standard engine (0% H_2O), the decreasing of temperature is about 5.5%; 14.75%; 26.57% and 40.9% for 20% H_2O; 40% H_2O; 60% H_2O and 80% H_2O respectively, using isooctane as a fuel. However, for HCCI fuelled with ethanol, compared to the standard engine (0% H_2O), the decreasing of temperature is about 5.84%; 15%; 26.64% and 39.84% for 20% H_2O; 40% H_2O; 60% H_2O; and 80% H_2O respectively.



(a)

(b)

Fig. 9 (a) Mean temperature variation with steam injection ratio using ethanol as a fuel (b) Mean pressure variation with steam injection ratio using ethanol as a fuel

Fig. 9 (b) denotes that increasing the steam injections worsen the cylinder pressure of the engine. On average, the cylinder pressure decreased by 8.48%; 19.98%; 33.48%, and 49.17% for respectively 20% H_2O; 40% H_2O; 60% H_2O, and 80% H_2O, using isooctane as a fuel. Then for ethanol, the cylinder pressure decreased by 7.85%; 19.41%; 32.7%, and 47.27%.

Fig. 10 shows the variation of ignition timing with steam injection and there for ethanol and isooctane respectively. Those results are usually obtained with a CR of 18 in a stoichiometric mixture. It appears that the Steam Injection has a small influence on the ignition timing and especially for isooctane. We can note that for water vapor injection greater than 40% for ethanol or 30% for isooctane, there is no effect of steam injection on the ignition timing.

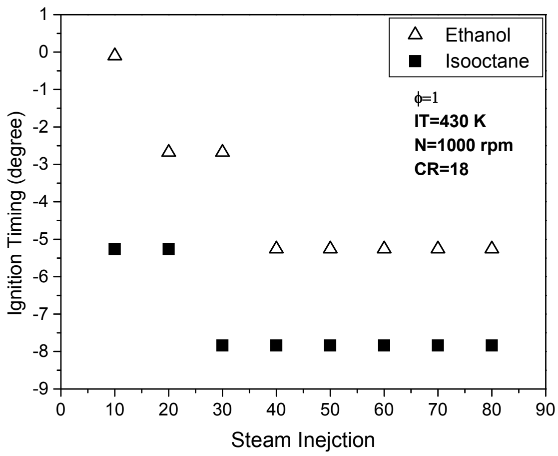


Fig. 10 Effect of Steam Injection on the ignition timing of HCCI engine

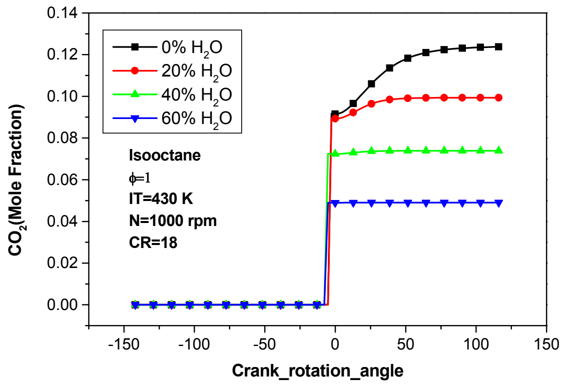


Fig. 11 Variation of CO_2 mole fraction versus CR, using isooctane as a fuel

2. Engine Emission Studies

Emission of different exhaust gas species (CO_2, and CO) with varying steam injection is presented in this section. The comparison of CO_2 emissions of steam injected and standard HCCI engine is shown in Figs. 11 and 12. It is to note that the CO_2 emissions reduce with steam injection for the two fuels.

Figs. 13 and 14 show the CO emissions for different steam ratios using isooctane or ethanol as a fuel respectively. In this case, the injection of SI can reduce significantly the CO emission. Carbon monoxide, CO, is emitted as a result of incomplete combustion of carbon and oxygen under high temperature inside the cylinder. It's clear from these figures that the water vapor injection caused a reduce in CO emissions.

E. Compression Ratio (CR)

1. Effect on Ignition Timing

In this section of search, we will concentrate on the effect of CR on Ignition timing. The CR is defined as the ratio of the maximum cylinder volume to the minimum volume. Figs.15 and 16 illustrate the variation of temperature and the pressure obtained for different values of CR on the HCCI Engine Operation Fuelled with Ethanol. These figures indicate that increasing the CR; the ignition is retarded; the burn duration is decreased, and the in-cylinder heat release and chemical reaction rates are enhanced. As a result, the maximum pressure and temperature go up. Many CR shaves have been tested numerically, and combustion process cannot occur for the CR lower than 16.

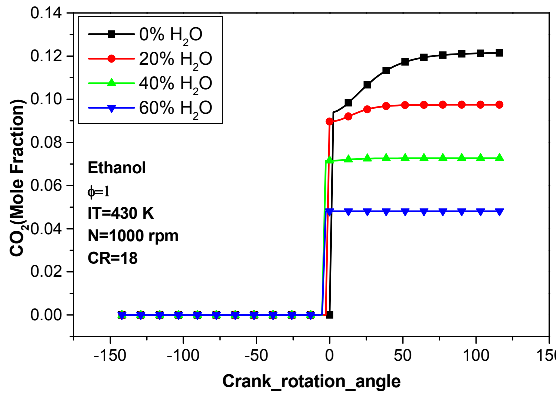


Fig. 12 Variation of CO_2 mole fraction versus CR, using ethanol as a fuel

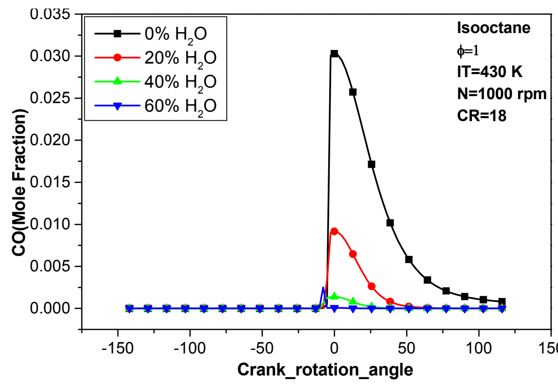


Fig. 13 Variation of CO mole fraction versus CR, using isooctane as a fuel

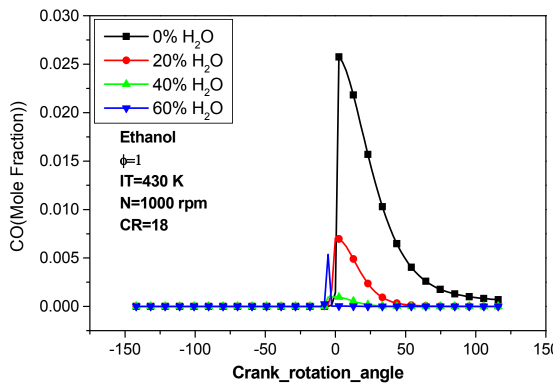


Fig. 14 Variation of CO mole fraction versus CR, using ethanol as a fuel

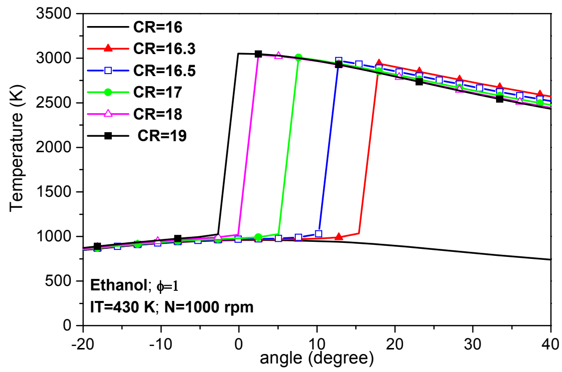


Fig. 15 Variation of temperature versus crank angle for different CR using ethanol as a fuel

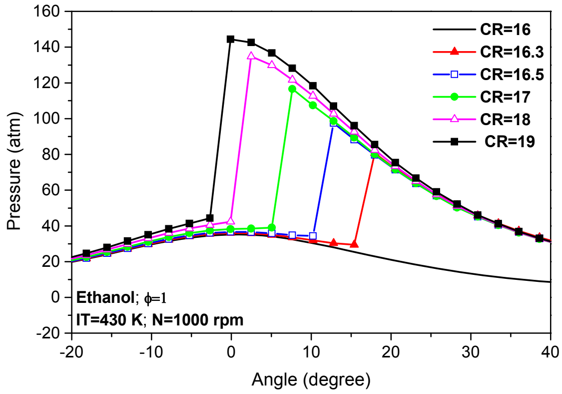


Fig. 16 Variation of pressure versus crank angle for different CR, using ethanol as a fuel

Temperature and pressure profiles obtained for different values of CR, using isooctane or ethanol as a fuel in an equivalence ratio equal to 1, are plotted in Figs. 17 and 18. Different CRsare tested in this case, and it demonstrates that when CR is high, the ignition can be reached more easily.

Fig. 19 depicts the effect of CR on ignition timing obtained from the data presented in Figs. 15 and 16 for ethanol and from the data presented in Figs. 17 and 18 for isooctane respectively. Those results show that the relationship between CR and its effect on HCCI combustion ignition timing is non-linear, but high values of CR, in general, results in earlier combustion initiation. It also shows that with a minimum value of CR exists, 16 for ethanol, below it, ignition timing becomes infinite and no combustion occurs but for isooctane, a critical minimum value of CR is 14. This figure demonstrates that using a CR greater than 21, have not an effect on ignition timing and there with using isooctane or ethanol as a fuel.

2. Engine Emission Studies

The effect of CR on CO_2 emission is shown in Figs. 20 and 21 using isooctane or ethanol as a fuel respectively. The CO_2 emission increases by increasing the CR. The rise of CR leads to a high temperature and pressure which increases CO_2. This numerical study demonstrates that with a CR equal to 19 a maximum CO_2 emission has been reached. However, the lowest emission of CO_2 has been reached with CR equal to 14 for isooctane and CR equal to 16.2 for ethanol.

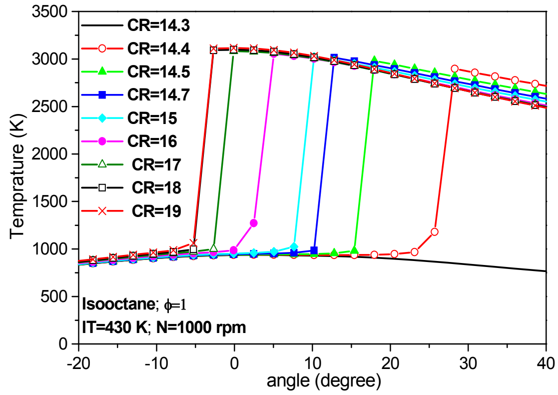


Fig. 17 Variation of temperature versus crank angle for different CR, using isooctane as a fuel

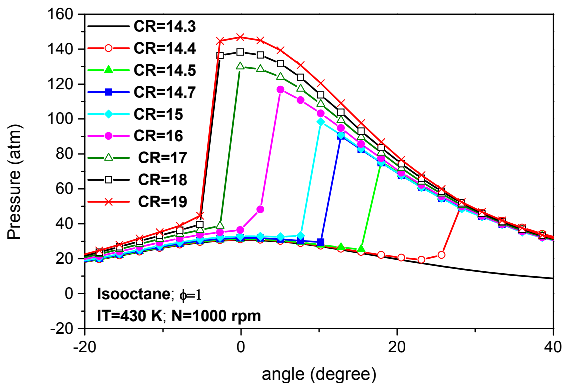


Fig. 18 Variation of pressure versus crank angle for different CR, using isooctane as a fuel

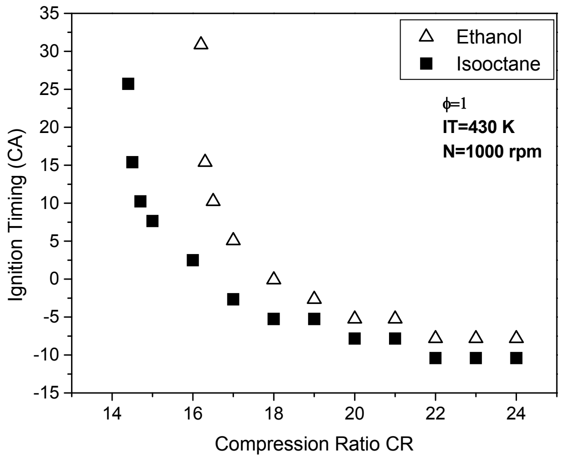


Fig. 19 Effect of CR on the ignition timing of HCCI engine

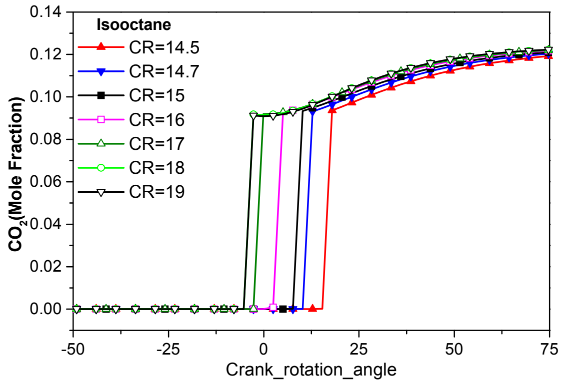


Fig. 20 Variation of CO_2 mole fraction versus CR, using isooctane as a fuel

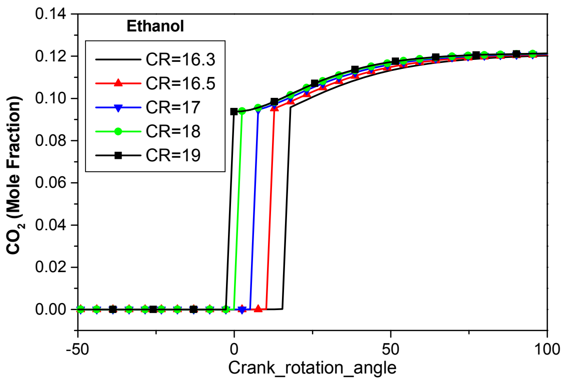


Fig. 21 Variation of CO_2 mole fraction versus CR, using ethanol as a fuel

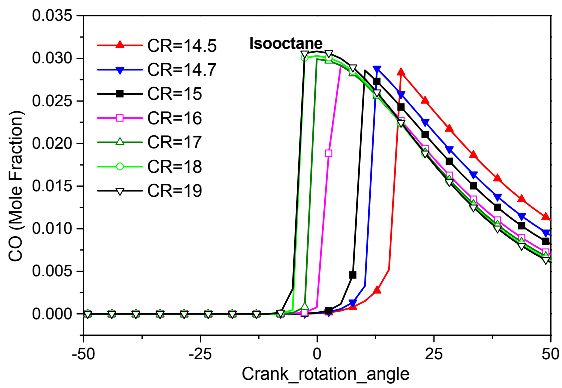


Fig. 22 Variation of CO mole fraction versus CR, using isooctane as a fuel

Variations of CO emission obtained for different CRs are plotted in Figs. 22 and 23 and the by using isooctane or ethanol as a fuel respectively. Those figures clearly show that the CO emission increased by increasing CRs.

IV. Conclusion

In this study, a thermodynamic model is used to predict and analyze the combustion of HCCI. The effects of the variable type of fuel used on the ignition timing and emissions characteristics of HCCI engine are observed. Combustion simulations of isooctane and ethanol with air in ICE have been performed. Then, emission of different exhaust gas species (CO_2, and CO) with varying operating conditions such as CRsand steam injection is presented.

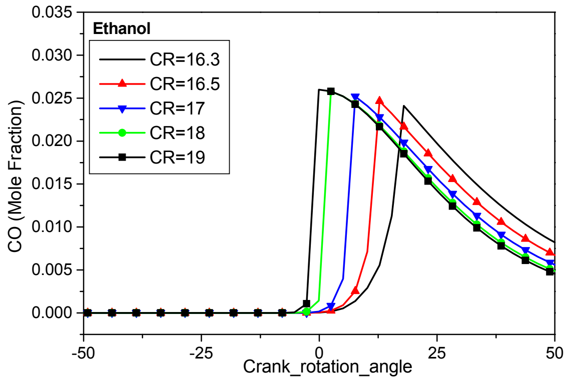


Fig. 23 Variation of CO mole fraction versus CR, using ethanol as a fuel

Based on the numerical study, the following results were obtained:

- Two different fuels have been tested in this study: isooctane (IC_8H_{18}), and ethanol (C_2H_5OH). We concluded that isooctane ignited more easily than ethanol. It can be explained by the effect of the octane numbers: fuels with lower octane numbers (isooctane) are ignited more easily.
- Many CRs have been tested numerically, and the combustion process cannot occur for the CR equal and lower than 14 and 16 for HCCI engine fuelled with isooctane or ethanol respectively in a stoichiometric mixture: when the CR of 16 for ethanol and 14 for isooctane, the highest temperature of the cylinder did not reach the desired temperature by the low-temperature reaction did not occur on fire.
- For CR greater than 21, the effect of CR on ignition timing becomes negligible for the two fuels.
- With the increase in CR, the temperature reached is also high, and the ignition timing is so advanced but, this effect increased the pollutant emissions. However, the lowest emission has been obtained with CR equal to 14 for isooctane and CR equal to 16.2 for ethanol.
- A suitable choice of CR ensuring HCCI ignition near TDC plays an important role. In this study, we pick out a CR equal to 17 for isooctane and 18 for ethanol in terms of performance and emission parameters.
- Keep the other parameters constant, respectively, the steam injection is set to: 0%; 20%; 40%; and 60% H_2O. For water vapor injection greater than 40% for ethanol and 30% for isooctane, there is no effect of steam injection on the ignition timing.
- The cooling effect of steam injection lowers in-cylinder peak temperatures and provides lower pollutant emission values.

- Numerical results show that 20% seems as optimum steam injection ratio in terms of pollutant emissions reduction without a loss in performance.

Other means of ignition control can also be used for HCCI combustion, such as intake temperature and intake pressure, and the study of these controls is recommended for future work.

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