

# Effect of Hydrogen Addition to Natural Gas on Homogeneous Charge Compression Ignition Combustion Engines Performance and Emissions Using a Thermodynamic Simulation

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## Abstract

The HCCI combustion process is initiated due to auto-ignition of fuel/air mixture which is dominated by chemical kinetics and therefore fuel composition has a significant effect on engine operation and a detailed reaction mechanism is essential to analysis HCCI combustion. A single zone-model permits to have a detailed chemical kinetics modeling for practical fuels. In this study a single-zone thermodynamic model with detail chemical mechanism is developed to investigate the effect of hydrogen addition to natural gas in a homogeneous charge compression ignition combustion and to analyze the performance and emissions of the HCCI engine. The effect of five different percentage of hydrogen added to natural gas ranging from 0 to 40 on HCCI combustion is investigated in this study. The results indicate that by increasing hydrogen portion in intake mixture, start of combustion advances and maximum temperature increase, but increasing in maximum pressure is negligible. Carbon's included emissions such as Co, Co<sub>2</sub> and unburned hydrocarbons decreases by increasing of hydrogen, and also, specific fuel consumption decreases. The result shows that hydrogen improves combustion characteristics of natural gas in an HCCI engine and leads to better performance and less emissions.

*Keywords: HCCI Combustion, Hydrogen, Natural Gas, Thermodynamic Simulation*

## 1. INTRODUCTION

Internal combustion engines are widely used for power generation including automotive and industrial applications. Although significant progress in engine technologies are achieved in recent years, however still major challenges about emissions and long term availability of petroleum fuels are of concerns. For resolving these issues the new combustion mode of homogeneous charge compression ignition (HCCI) is presented [1]. In HCCI combustion, a lean air-fuel mixture and recirculated combustion products are auto-ignited during compression stroke [2]. Unlike spark-ignition (SI) engines, where ignition is initiated by the spark, and CI engines which it is initiated by auto-ignition of injected fuel at its interface with in cylinder charge, in HCCI mode the auto-ignition of the mixture depends on its thermo chemical properties and the local flow conditions [3,4] and it occurs simultaneously at many locations throughout the combustion chamber without any flame propagation

[1, 5 and 6]. HCCI combustion displays a peculiar two-stage heat release just like diesel where the initial stage is associated with low temperature kinetic reactions and the later depends on high temperature. The time delay between stages is associated with the “negative temperature coefficient (NTC) regime” [7,8].

The HCCI concept was initially investigated by Onishi et al. [1] in 1979 to improve gasoline fuel combustion stability in a two-stroke engine. The achievement was major fuel and emissions reduction by creating conditions to have spontaneous ignition of in-cylinder charge with stable HCCI combustion within low and high load limits for an engine with compression ratio of 7.5:1 and speeds ranging from 1000 to 4000 rpm. Najt and Foster in 1983 [9] extended the idea to a four-stroke engine and attempted to get a better understanding of the physics behind HCCI combustion. It is an accepted fact that HCCI auto-ignition below 1000 K is controlled by low temperature mechanism but the main energy release is

controlled by high temperature mechanism above 1000 K which results in further oxidation of CO. The major advantage of homogeneous charge compression ignition engines is its potential for higher thermal efficiency together with its capabilities to reduce soot and NO<sub>x</sub> [10]. Despite all these benefits there are some operational issues due to the lack of accurate controllability of ignition and combustion at certain load and speed. Also HC and CO concentration could increase in exhaust gases due to relatively cold in-cylinder regions especially in the crevices and thermal boundary layer [10–17].

Different models have been developed from multi-dimensional [18], multi-zone [20] and single-zone models in an effort to improve our understanding of HCCI combustion and a better description of its features. Fiveland and Assanis [19] constructed a two-zone HCCI model by dividing the combustion chamber into an adiabatic core and a thermal boundary layer zone. In this model mixing of zones is permitted and the thermal boundary layer thickness was calculated for a complete cycle using a simple heat transfer model. Easley et al. [20] used a six zone model to describe the physical processes during combustion; having three adiabatic core zones without any mass transfer and the outer core zone which is permeable to mass with the boundary layer zone and a fixed crevice zone. In this model thermal boundary layer thickness is assumed to be constant since there is not any considerable heat or mass transfer between zones. The combustion process is modeled using chemical kinetics for a set of chemical reactions and the combustion chamber's temperature and mass distribution is estimated at IVC for initialization of combustion process. It is highlighted that the crevice regions and the boundary layer have an impact on unburned HC and CO emissions. Similar nine zones model was used by Ogink and Golovitchev [21] with estimated temperature–volume fraction distribution at IVC and a fixed thermal boundary layer thickness during compression and expansion strokes. For simplicity heat and mass transfer between all zones has been excluded from calculation which this of course could affect the accuracy of combustion mechanism and also distribution of CO and unburned HC emissions. Xu et al. [22] also used similar scheme introduced by Easley et al., again by neglecting heat and mass transfer between zones which leads to underestimated CO and overestimated HC emissions.

In order to understand better the auto-ignition process in an HCCI engine, the influence of some important parameters on the auto-ignition is investigated by H. Machrafi et al. [23]. The inlet temperature, the equivalence ratio and the compression ratio were varied and their influence on the pressure, the heat release and the ignition delays were measured. The chemical behavior of three different fuel surrogates, containing n-heptane, iso-Octane, toluene, and 1-pentene, under HCCI conditions is analyzed by M. Mehl et al. [24]. New experimental measurements of the in-cylinder composition have been carried out on a running HCCI engine equipped with a special customized cylinder head allowing the direct sampling of the gas.

H. Machrafi et al. in 2008 investigated the possibility of using gasoline in an HCCI engine and analyzed the auto-ignition of gasoline in such an engine. For comparison, a PRF95 and a surrogate containing 11 vol% n-heptane, 59 vol% iso-Octane, and 30 vol% toluene were used. A previously validated kinetic surrogate mechanism was used to analyze the experiments and to yield possible explanations to kinetic phenomena. Their results showed that it is quite possible to use the high Octane-rated gasoline for auto-ignition purposes, even under lean inlet conditions [25].

Because of dominant role of chemical kinetics in HCCI combustion, it is important to have a good understanding of reaction mechanisms of hydrocarbon fuels in order to correctly interpret experimental data and putting HCCI engine development in a right pass. A comprehensive HCCI combustion model should consider fluid mechanics, heat transfer interaction and detailed kinetics aspect of the process [26]. The computational fluid dynamics (CFD) could study the HCCI combustion of simple fuels, but it is often computationally too time consuming to analyze the case of practical fuels. Single-zone HCCI combustion models, on the other hand, permit detailed modeling of the chemical kinetics for practical fuels by assuming that the gas in the combustion chamber is homogeneous also the temperature, pressure and gas composition are uniform. This model can adequately predict ignition in HCCI engine when initial conditions are known. This model could be the best approach when time is important or there is computational limitation.

In this study a thermodynamic single-zone model

with detailed chemical kinetic is used to investigate the effect of hydrogen on HCCI combustion of natural gas. This model assumes that fuel/air mixture homogenously propagates in combustion chamber and considers combustion chamber a single-zone in which pressure, temperature and fuel composition is uniform. Only the closed cycle part of the engine (namely the period between the time of closing intake valve and opening exhaust valve) is modeled. The present work is modeled by means of a detailed chemical kinetic reaction mechanism proposed by Dagaut. [27], which was validated previously by experimental data and includes 97 species involved in 732 reversible reactions. In the present study, specific heat capacity, entropy and enthalpy of species have been calculated from 7-order polynomials that extracted from NASA table [28]. The conservation of mass, energy, and gas-phase species equations are solved and pressure, temperature distributions, mole fraction of species, CO, CO<sub>2</sub> and unburned hydrocarbons emissions in each time step are calculated. Also specific fuel consumption and start of combustion are obtained for each case. In this work, the simulation is done for a four valves per cylinder engine and initial conditions are bore of 81.6 mm, stroke of 88.2 mm, compression ratio of 15.0, pressure at IVC of 105 Pascal, and revolutions per minute (RPM) of 1500. Heat transfer from wall is calculated using Woschni [28] heat transfer equation. Wall temperature is considered 1500C.

## 2. GOVERNING EQUATIONS

### 2. 1. Conservation of Mass and Energy

Combustion chamber is considered as a closed system with no mass crossing the boundary, therefore total mass of the mixture  $m = \sum_{k=1}^K m_k$  is constant and  $dm/dt = 0$ . Here  $m_k$  is the kth specie's mass and K the total number of species. Considering that  $Y_k = m_k/m$  is the mass fraction of the kth species, the general conservation of mass and in the form of production and destruction of individual species are as follows; respectively:

$$\frac{dY_k}{dt} - \nu \dot{\omega}_k W_k = 0 \quad , \quad \frac{dY_k}{dt} = \nu \dot{\omega}_k W_k$$

Where  $\nu = V/m$  is the specific volume, which may vary with time t and  $\dot{\omega}_k$  is the molar production

rate of the kth species due to elementary reaction also  $W_k$  is the molecular weight of the kth species.

The net chemical production rate  $\dot{\omega}_k$  of each species is the balance of its production and consumption within chemical reactions involving that species. Each reaction takes place according to forward and backward coefficient rates defined by k, which is obtained from modified Arrhenius equation;

$$k_i = A_i T^{\beta_i} \exp\left(\frac{-E_i}{R_c T}\right)$$

Where  $A_i$  is the pre-exponential constant,  $\beta_i$  is the temperature exponent and  $E_i$  is the activation energy for reaction i, and these parameters are included in chemical mechanism.

The energy equation for inner zones is;

$$\rho C_v \frac{dT}{dt} + \frac{P}{V} \frac{dV}{dt} + \sum_{k=1}^K u_k \dot{\omega}_k W_k = 0$$

While for boundary layer and crevice zones with wall heat transfer, becomes;

$$\rho C_v \frac{dT}{dt} + \frac{P}{V} \frac{dV}{dt} + \sum_{k=1}^K u_k \dot{\omega}_k W_k + \frac{h_w(T - T_w)A_w}{V} = 0$$

Where  $C_v = \sum_{k=1}^K m_k C_{v,k}$  is the specific heat capacity of gas mixture at constant-volume; P, T, and V are zone pressure, temperature and volume respectively,  $u_k$  is the internal energy of the k<sub>th</sub> species and  $h_w$  and  $A_w$  are zone wall heat transfer coefficient and surface area; respectively. The pressure is derived through ideal gas equation of state:

$$p = \frac{\rho RT}{\bar{W}}$$

Where R is the universal gas constant,  $\bar{W}$  is the mixture mean molecular weight and  $\rho$  is the mass density.

### 2. 2. Wall Heat-Transfer

Convective heat loss during compression and expansion strokes to the walls at each time step is derived by;

$$Q_{wall} = hA(T - T_{wall})$$

Where h is heat transfer coefficient and is obtained from the following generalized heat transfer

formulation based on user-specified constants of a, b and c which could be obtained from experimental data. For Woschni correlation (2003) which is widely used in internal combustion engine simulation a, b and c are 0.035, 0.8 and 0; respectively.

$$Nu_h = aRe^bPr^c$$

### 3. RESULT AND DISCUSSION

The simulated in cylinder temperature and pressure versus crank angle are shown in figures 1 and 2. As it is shown, hydrogen addition to natural gas, advanced combustion and increases in cylinder maximum

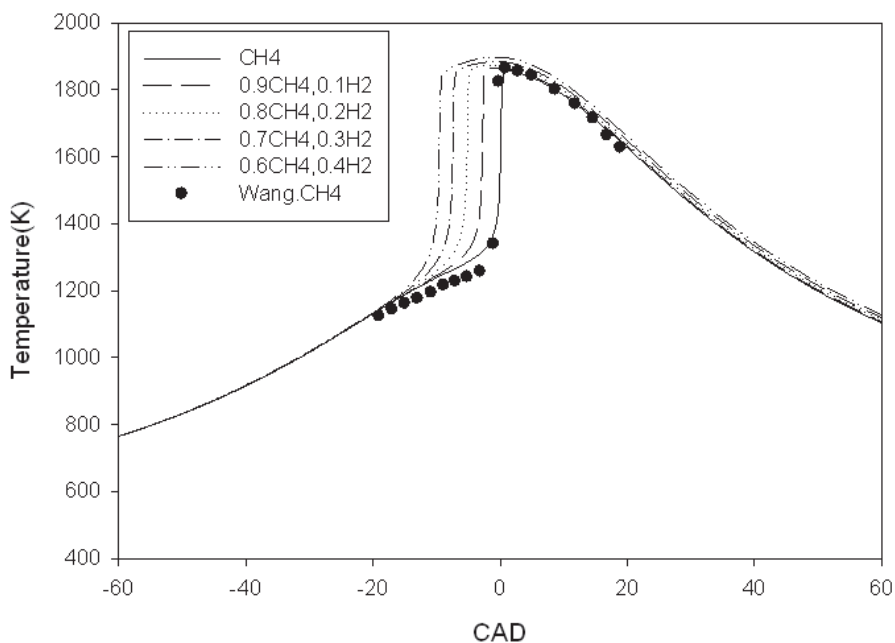


Fig. 1. Effect of hydrogen addition on cylinder temperature

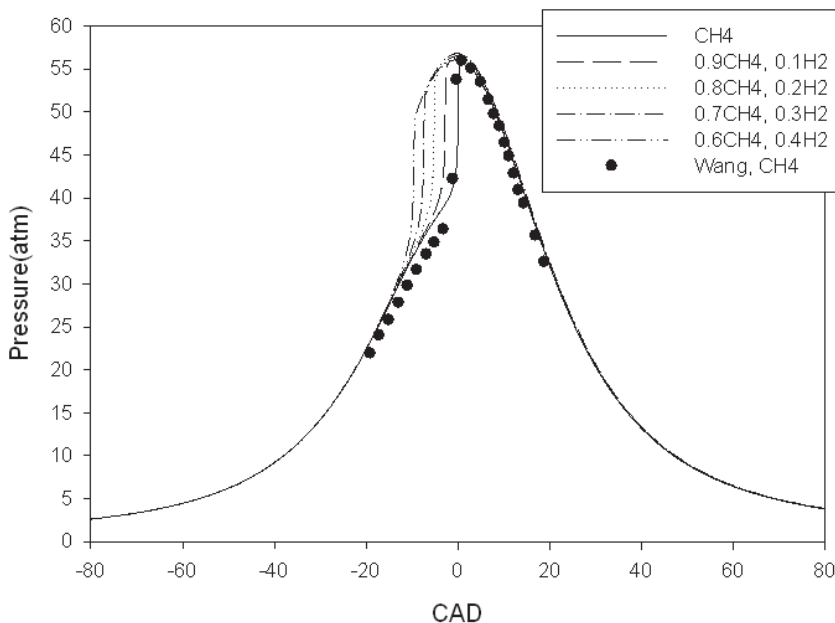


Fig. 2. Effect of hydrogen addition on cylinder pressure

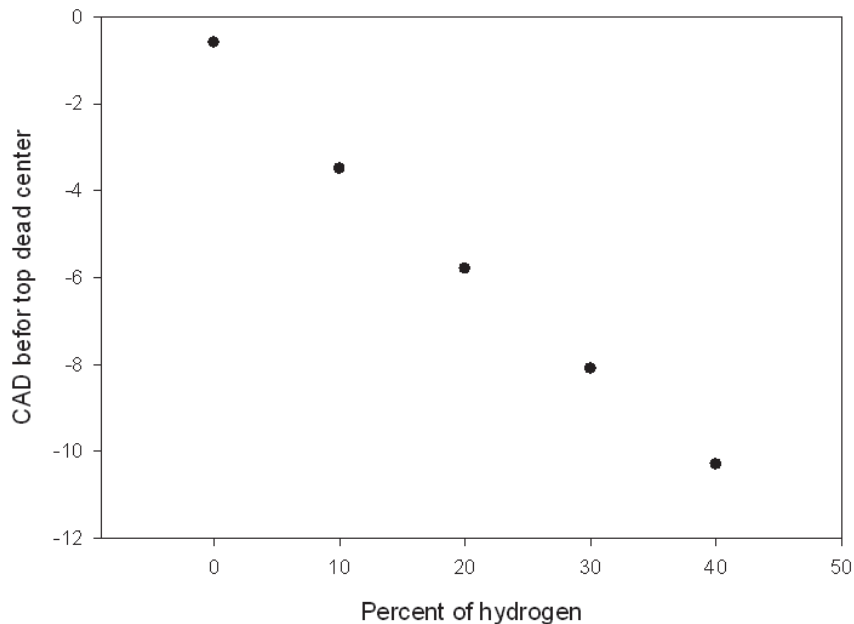


Fig. 3. Effect of hydrogen addition on start of combustion

temperature, but its effect on maximum pressure is negligible. This is due to hydrogen low motor octane number (MON), which causes its less resistance to auto-ignition rather than natural gas. The results are compared with the results of Z. Wang et al[29]. for natural gas combustion which shows good agreement. The effect of hydrogen addition to natural gas on calculated start of combustion is shown in Fig 3. By addition 10 percent hydrogen to natural gas, start of

combustion advances approximately 3 crank angle degree (CAD), and by increasing share of hydrogen to 40 percent, start of combustion advances around 10 CAD, which shows remarkable effect of hydrogen addition on advancing start of combustion which is due to its low motor octane number.

The result for calculated  $Co$ ,  $Co_2$  and unburned hydrocarbons are shown in figures 4 to 7. As it is shown in Fig 4, hydrogen addition does not have any

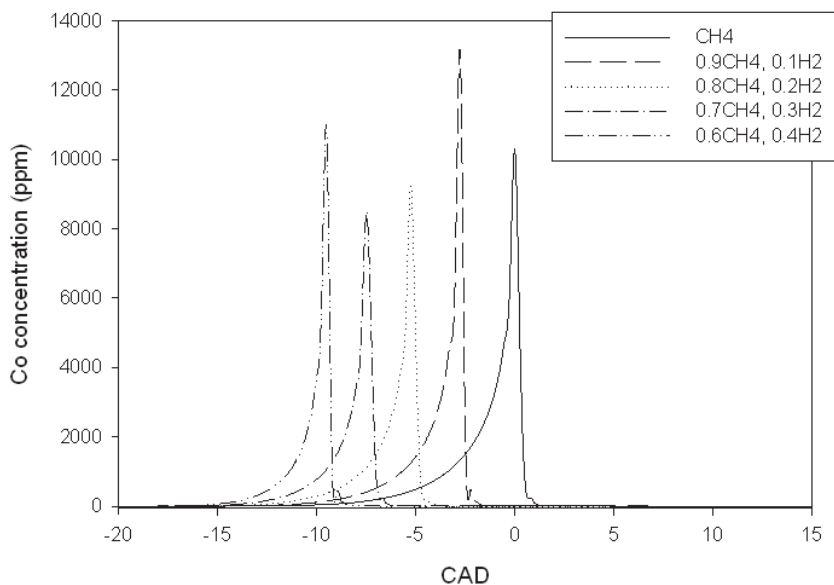


Fig. 4. The effect of hydrogen addition on CO concentration

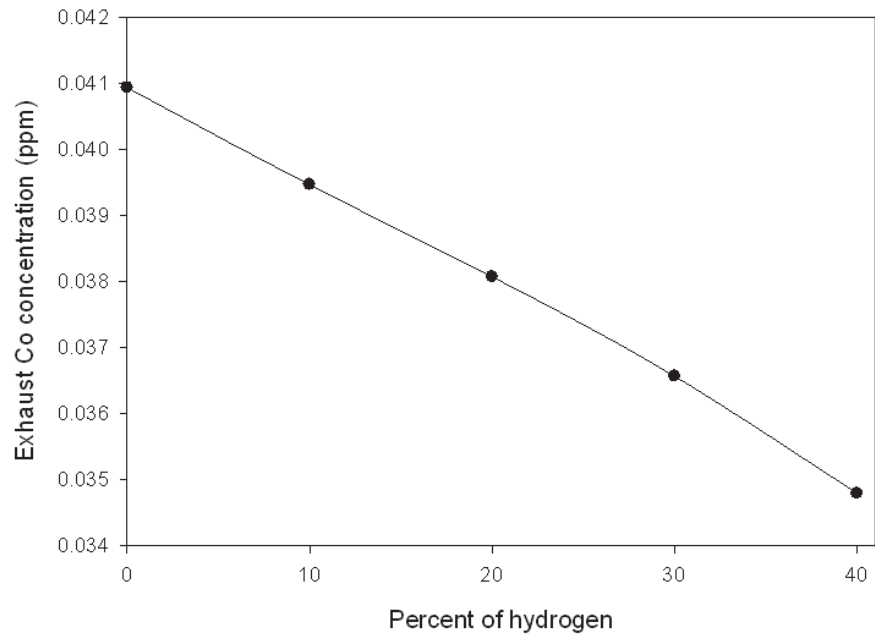


Fig. 5. The effect of hydrogen addition on exhaust CO

specific effect on maximum concentration of Co, but by increasing the amount of hydrogen the spread of Co production becomes narrower and its production starts sooner. As it is shown in figures 5, 6 and 7, exhaust Co, Co<sub>2</sub> and unburned hydrocarbons decreases by increasing hydrogen portion in intake mixture. This is because of fixed intake pressure and temperature in all cases which means that the volume of intake mixture

is the same in all cases, and as a result, by increasing hydrogen portion in intake mixture the mass of natural gas and therefore carbon molecules in the intake mixture decreases which lead to decrease in carbon included emissions. It is also obvious from Figs 6 and 7 that, increasing in hydrogen portion in intake manifold, advances the start of Co<sub>2</sub> production and unburned hydrocarbons.

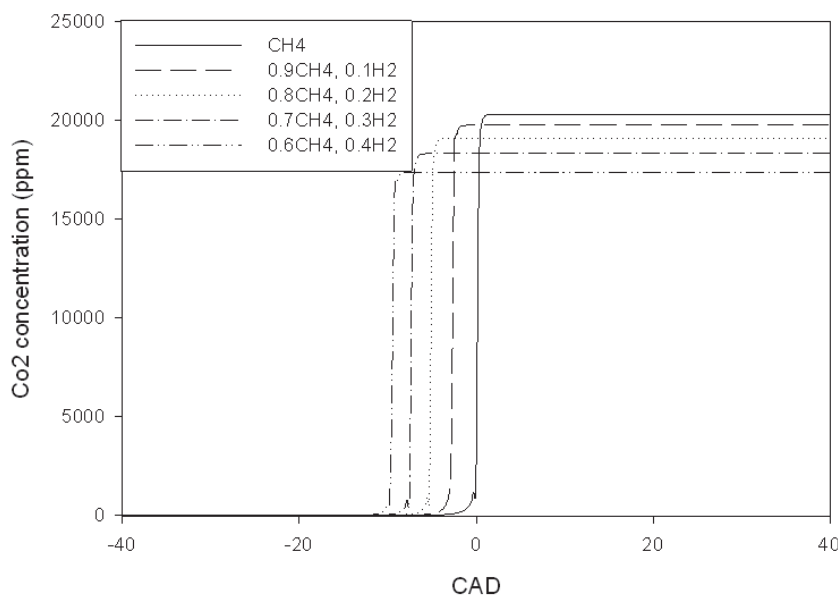


Fig. 6. The effect of hydrogen addition on CO<sub>2</sub> concentration



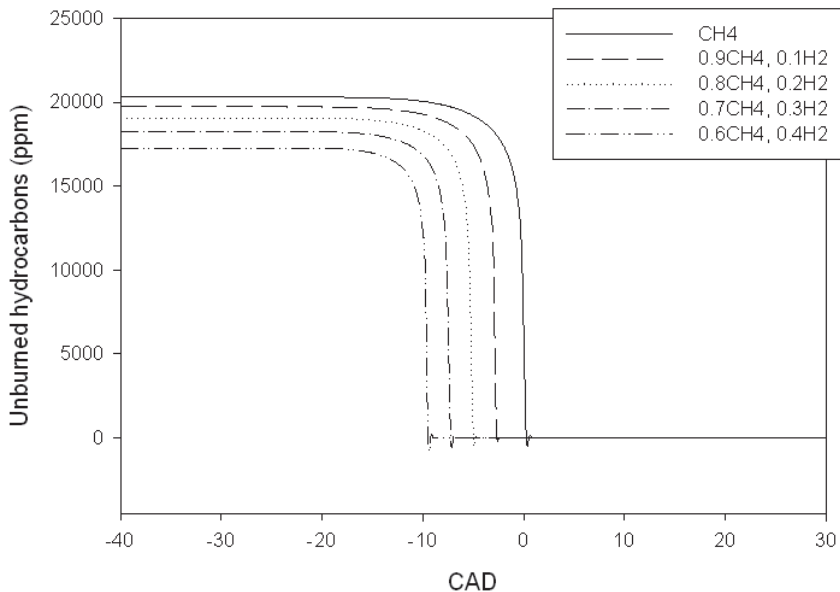
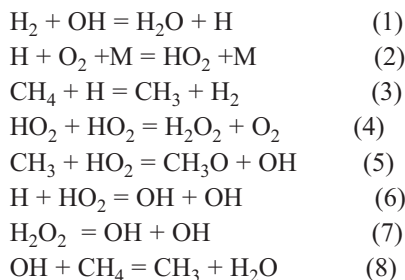


Fig. 7. Unburned Hydrocarbons concentration(ppm) versus crank angle

The effect of hydrogen addition on specific fuel consumption is shown in Fig. 8. As it is shown, the increase in hydrogen amount decreases the ISFC. This could be due to two folds; hydrogen has a smaller molecular weight comparing to natural gas and performs a more complete combustion which ends up with higher heat release.

Brief analysis of the chemical kinetics will provide a better understanding of the combustion process. The important reactions in CH<sub>4</sub>-H<sub>2</sub> combustion are listed below [27]:



Net reaction rates of these important reactions for combustion of CH<sub>4</sub> with 20% of H<sub>2</sub> are shown in Fig.

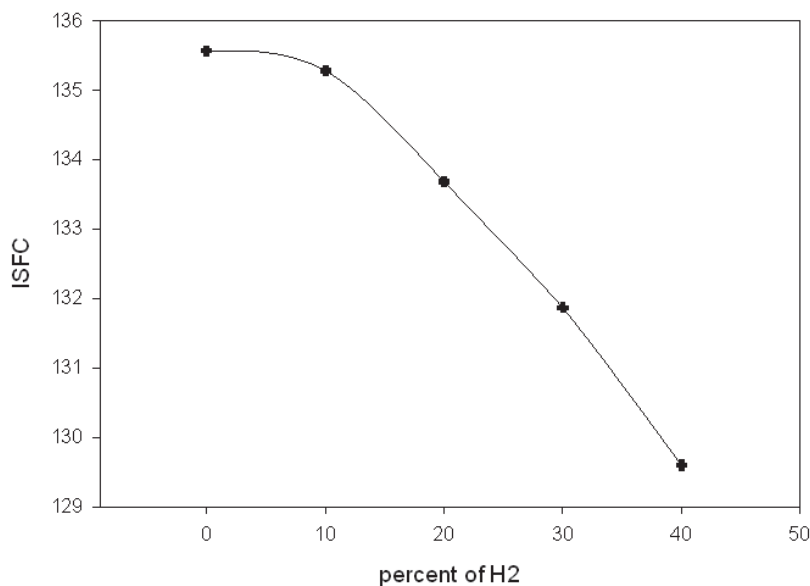


Fig. 8. Effect of hydrogen addition on indicated specific fuel consumption

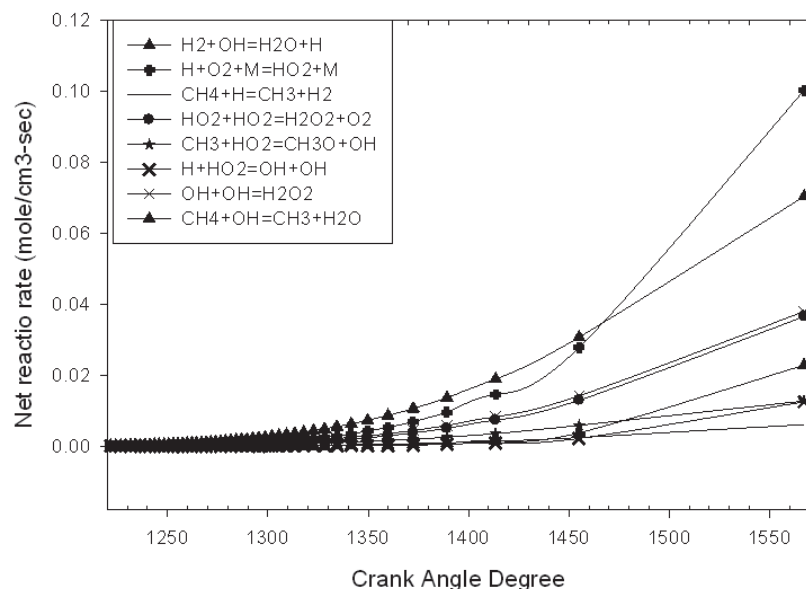


Fig. 9. Net reaction rate of important reactions

9. As is shown, reaction 8 is the most effective reaction for consumption of  $\text{CH}_4$ , which means OH is the most crucial species for increasing or decreasing combustion rate of  $\text{CH}_4$ . As is shown in reaction 1 through 8,  $\text{H}_2$  addition leads to an increase in radical H according to reaction (1). H contributes to the production of  $\text{HO}_2$  and  $\text{CH}_3$  via reactions (2) and (3) respectively.  $\text{HO}_2$  partially converts to  $\text{H}_2\text{O}_2$  via reaction (4).  $\text{CH}_3$ ,  $\text{HO}_2$  and  $\text{H}_2\text{O}_2$  are crucial radicals and they promote the formation of OH via reactions

(5), (6), and (7). OH plays a crucial role in the oxidation of  $\text{CH}_4$  via reaction (8). Thus  $\text{H}_2$  addition leads to more OH radicals, the ignition is advanced, and the temperature and the pressure are enhanced. The mole fraction of OH for different studied cases is shown in Fig. 10. As is shown, by increasing  $\text{H}_2$  the OH production advances and its mean value increases which leads to advance in start of combustion. The maximum amount of OH mole fraction is not reliable, because it occurs in a short window of time which may

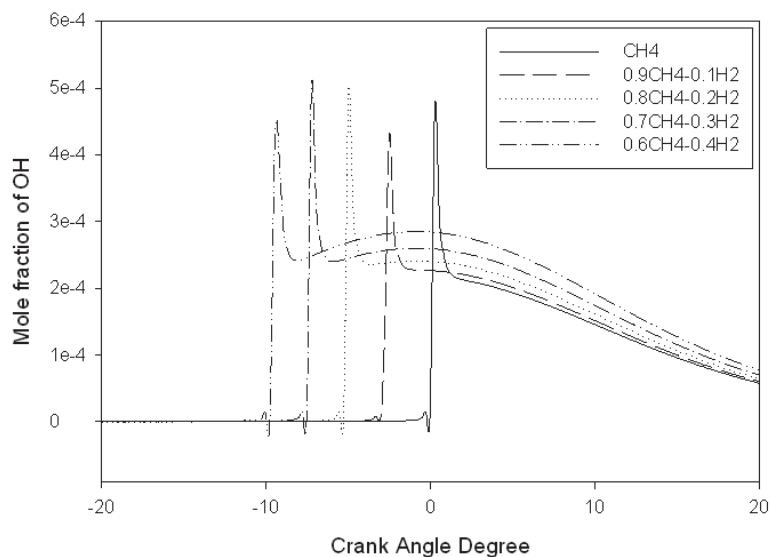


Fig.10. Effect of addition of  $\text{H}_2$  to  $\text{CH}_4$  on radical OH



be due to rapid increase in pressure in single zone modeling.

#### 4. CONCLUSION

A thermodynamic single-zone model with a detail chemical kinetic mechanism is used to model the combustion of five different blended natural gas and hydrogen fuels in an HCCI engine. The chemical kinetic mechanism that has been used in this work includes 732 reactions. The results of the simulations can be summarized as the following:

- Hydrogen addition to natural gas improves HCCI combustion characteristics namely; less emissions and better performance.
- Since hydrogen is a lighter fuel rather than natural gas, its addition to natural gas increases peak pressure and temperature, it also advances start of combustion.
- Increasing hydrogen portion in intake mixture from 0 to 40 percentages, advances start of combustion around 10 crank angle degrees.
- Hydrogen addition to natural gas decreases carbon included emissions.
- Hydrogen decreases ISFC, which means it releases much energy than natural gas with the same weight.
- Blending two fuels with different characteristics can improve HCCI combustion performance and emissions.

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