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# Investigation the effect of hydrogen addition on the ignition timing in the methane-fuel HCCI engine

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## Abstract

Homogeneous charge compression ignition (HCCI) is one of the alternatives to reduce significantly engine emissions for future regulations. This new alternative combustion process is mainly controlled by chemical kinetics in comparison with the conventional combustion in internal combustion engines. In this paper, the effect of $H_2$ addition on ignition timing of a natural-gas HCCI engines have been investigated numerically by adopting a single-zone zero-dimensional model. The chemical kinetic mechanism incorporated the GRI-3.0 mechanism that considers 53 species and 325 reactions together. To simulate HCCI engine cycles, a variable volume computation has been performed by including the piston motion into the chemical reaction design, CHEMKIN, code. The SENKIN code used in order to simulate the in-cylinder combustion. It was found that an additive-free mixture did not ignite for the intake temperature of 500 K. A mixture containing a small quantity of additives at the same temperature was ignited. For a fixed quantity of additive, it was found that $H_2$ addition was effective in advancing the ignition timing. It was also found that the percentage of additive required to achieve a near TDC ignition timing increases linearly with the increase in the engine speed while decreases with the increase in the equivalence ratio. Furthermore, the addition of 24% mass of $H_2$ could ignite a mixture at an intake temperature of 450 K.

Keywords: Homogeneous Charge Compression Ignition (HCCI), Chemical Kinetics, Methane-fuel, Additives.

## 1-Introduction

Strategy of the automobile industry implies developing new engines functioning with a low equivalence ratio, lower fuel consumption and consequently reducing $CO_2$, $NOx$ and particulate emissions. Using a premixed air-fuel mixture and a lean burn combustion process at lower temperatures, the HCCI combustion allows obtaining a higher thermal efficiency, low $NOx$ emissions and low particulate-matter emissions [1]. Contrary to diesel combustion, where turbulence during flame diffusion is of great importance or gasoline combustion with a flame front propagation, the auto-ignition phenomenon in an HCCI engine is mainly controlled by chemical kinetics.

Disadvantages of HCCI engines include: high hydrocarbon $(HC)$ and carbon monoxide $(CO)$ emissions, high peak pressures, high rates of heat release, reduced operating range, low maximum power, difficulty in starting the engine, and difficulty of control.

HCCI was identified as a distinct combustion phenomenon about 20 years ago. Initial papers recognized the basic characteristics of HCCI that have been validated many times since then: HCCI ignition occurs at many points simultaneously, with no flame propagation [2, 3]. Combustion was described as very smooth, with very low cyclic variations. Noguchi et al. also conducted a spectroscopic study of HCCI combustion [3]. Many radicals were observed, and they were shown to appear in a specific temporal sequence. In contrast, with spark-ignited (SI) combustion all radicals appear at the same time (probably distributed in the same spatial sequence through the flame front). These initial experiments were done in 2-stroke engines, with very high EGR. Since then, HCCI two-stroke engines have been developed to the point of commercialization for motorcycles [4]. HCCI motorcycle engines have higher fuel economy, lower emissions and smoother combustion than 2-stroke spark-ignited engines. However, HC and CO emissions out of the HCCI engine are still very high compared with the current automotive emissions standards. An

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improved version of the engine has been recently evaluated, which shows improvements in fuel economy and emissions [5].

Najt and Foster did the first HCCI experiment with a four-stroke engine. They also analyzed the process, considering that HCCI is controlled by chemical kinetics, with negligible influence from physical effects (turbulence, mixing). They used a simplified chemical kinetics model to predict heat release as a function of pressure, temperature, and species concentration in the cylinder [6]. Since then, a description of the HCCI process has gained acceptance. HCCI has been described as dominated by chemical kinetics, with little effect of turbulence. Crevices and boundary layers are too cold to react, and result in hydrocarbon and CO emissions. Combustion at homogeneous, low equivalence ratio conditions results in modest temperature combustion products, which do not generate $NO_x$ or particulate matter.

Analysis of HCCI engines is not well developed, even though the process may be reasonably well understood. For homogeneous charge engines, the process is mainly dominated by chemistry, and it is more important to have a detailed chemical kinetics model than a fluid mechanics model. Therefore, valuable predictions and results can be obtained from single-zone chemical kinetics analyses that assume that the combustion chamber is a well-stirred reactor with uniform temperature and pressure [7, 8]. The ideal tool for HCCI analysis is a combination of a fluid mechanics code with a detailed chemical kinetics code. This is, however, beyond our current computational capabilities. The control of ignition timing could be also achieved either by addition of promoters (additives reducing ignition delay time) [9–12] or blending low cetane number fuels (such as natural-gas and methanol) with high cetane number fuels [13, 14].

The aim of the present work is to investigate the effect of $H_2$ addition the ignition timing of a natural gas HCCI engine. The effect of additive of hydrogen $(H_2)$ on the ignition timing is investigated numerically. As the HCCI combustion process is mainly dominated by chemistry with no requirements of flame propagation, the numerical study adopted detailed chemical kinetics, while neglected effects from transport phenomena.

## 2-Computational Model

Recent analytical developments support the view that HCCI combustion is dominated by chemical kinetics, and an analysis methodology based on this premise has had considerable success in predicting HCCI combustion and emissions.

A zero-dimensional detailed kinetic model is used here to model HCCI combustion. A premixed charge at uniform temperature and pressure is compressed and expanded at a rate that depends on the engine speed and geometry. The model described below is based on the assumptions that the mixture is a perfect gas, temperature and species concentrations are uniformly distributed. Needless to say, the cylinder contents are neither perfectly mixed, nor of uniform temperature. Albeit, single-zone simulations provide an excellent match with experimental results in terms of overall engine performance trends and particularly start of combustion prediction. In particular, the boundary layer, which contains significant amount of mass, must be at a lower temperature than the bulk gas near TDC. Due to the assumed temperature uniformity, our estimates of burn duration and the heat release processes will be shorter than in experiments. That is, the boundary layer and crevices will always react last and extend the heat release rate compared to this simulation. Single zone models also tend to over predict $NO_x$ due to the under prediction of heat release duration and the exponential dependence of $NO_x$ formation on temperature. Furthermore another weak point is an inability to precisely predict hydrocarbon and carbon monoxide emissions, which primarily depend on crevices and under prediction of the heat release duration by up to 50%. Despite these weaknesses, the speed and robust nature of the single-zone model make it an ideal tool for analyzing engine operating regimes. Since the aim of this study is basically to investigate the effect of different additives on the ignition timing of a natural-gas HCCI engine, the single-zone model can reasonably capture the relative effectiveness of various additives [14].

The model used here is based on a CHEMKIN chemical kinetics code [15]. This kind of model cannot capture the multi-dimensional processes that occur in a real engine cylinder, but, since the heat release is a global no propagating autoignition process, a zero-dimensional model can reasonably capture the start of combustion (autoignition) and heat release of the core mixture. Since the start of combustion of the central core dictates the overall process, control of this combustion timing will control performance. In the present study, one chemical kinetics schemes for natural-gas has been used. The natural-gas chemistry was

described by the GRI-3.0 mechanism that considers 53 species and 325 reactions, including $NO_x$ chemistry and was used to study the effect of $H_2$ addition [16].
The governing equation for piston motion is [17]:

$$\frac{V}{V_c} = 1 + \frac{1}{2}(r_c - 1)[R + 1 - \cos\ \theta - (R^2 - \sin^2\theta)^{\frac{1}{2}}] \quad (1)$$

Where $V_c$ is the clearance volume, $r_c$ is the compression ratio, R is the ratio of connecting rod length to crank radius, and $\theta$ is the crank angle. A transition from time to crank angle and vise versa could be made as [17]:

$$t = \frac{\theta}{6N} \quad (2)$$

Where N is the engine speed in rpm.

The engine specifications assumed in this research are shown in Table 1 [18].

**Table 1-Specification of the engine**

| Engine Parameter | Value |
|---|---|
| Cylinder Bore | 100 mm |
| Connecting Rod to Crank Radius Ratio | 4.4 |
| Displacement Volume | 785.4 $mm^3$ |
| IVC | 96 BTDC |
| EVO | 126 ATDC |
| Engine Speed | 1000 RPM |
| Compression Ratio | 18 |

## 3-Results and discussion

The best promoters are additives that are able to increase the radical concentration without disappearing the induction stroke. Simulations have been done in order to investigate the effect of $H_2$ addition on the combustion in HCCI engine. The effect of this additive on combustion timing has been evaluated.

At first, computation performed in order to investigate the effect of addition of each additive on ignition of mixture of $CH_4 - Air$. The mass fraction of 5% of $H_2$ was used. The comparisons were done at the intake temperature of 510 K, the intake pressure of 1 atm and the equivalence ratio of 0.4. The pressure profile is shown in Fig. 1. It is clear that addition of $H_2$ has a noticeable effect on advancing the ignition timing in comparison with the condition that the additive free mixture was used. Furthermore, with addition of $H_2$, the start of ignition will be advanced to before of the TDC and this would be result in reduction of indicated thermal efficiency. It means that the amount of this additive must be adjusted (decreased) in order to have a near TDC ignition timing.

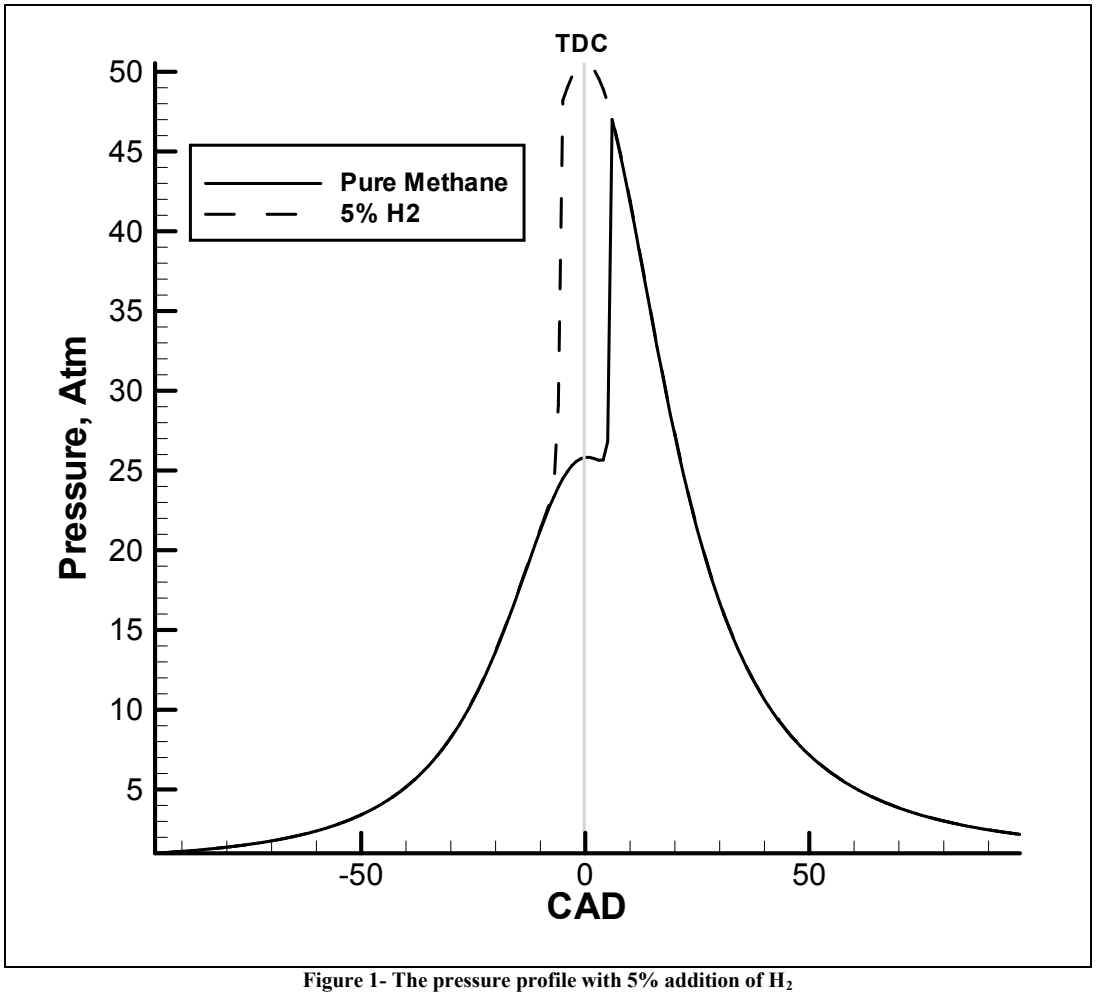


**Figure 1- The pressure profile with 5% addition of $H_2$**

In this regard, the computations were done to adjust the quantity of additives proper to achieve a near TDC ignition timing. The best combustion timing depends on different factors and varies depending on the operating conditions. The near TDC ignition timing is used as the best timing for combustion that provides a baseline for comparison of adequate mass fraction off each additive.

The effect of different amount of $H_2$ addition on the ignition timing is shown in Fig. 2. The computations were done at the intake temperature of 510 K, the intake pressure of 1 atm and the equivalence ratio of 0.4. It can be concluded that in order to reach the near TDC ignition timing, only a mass fraction of 1% of $H_2$ (Fig. 2) is required.

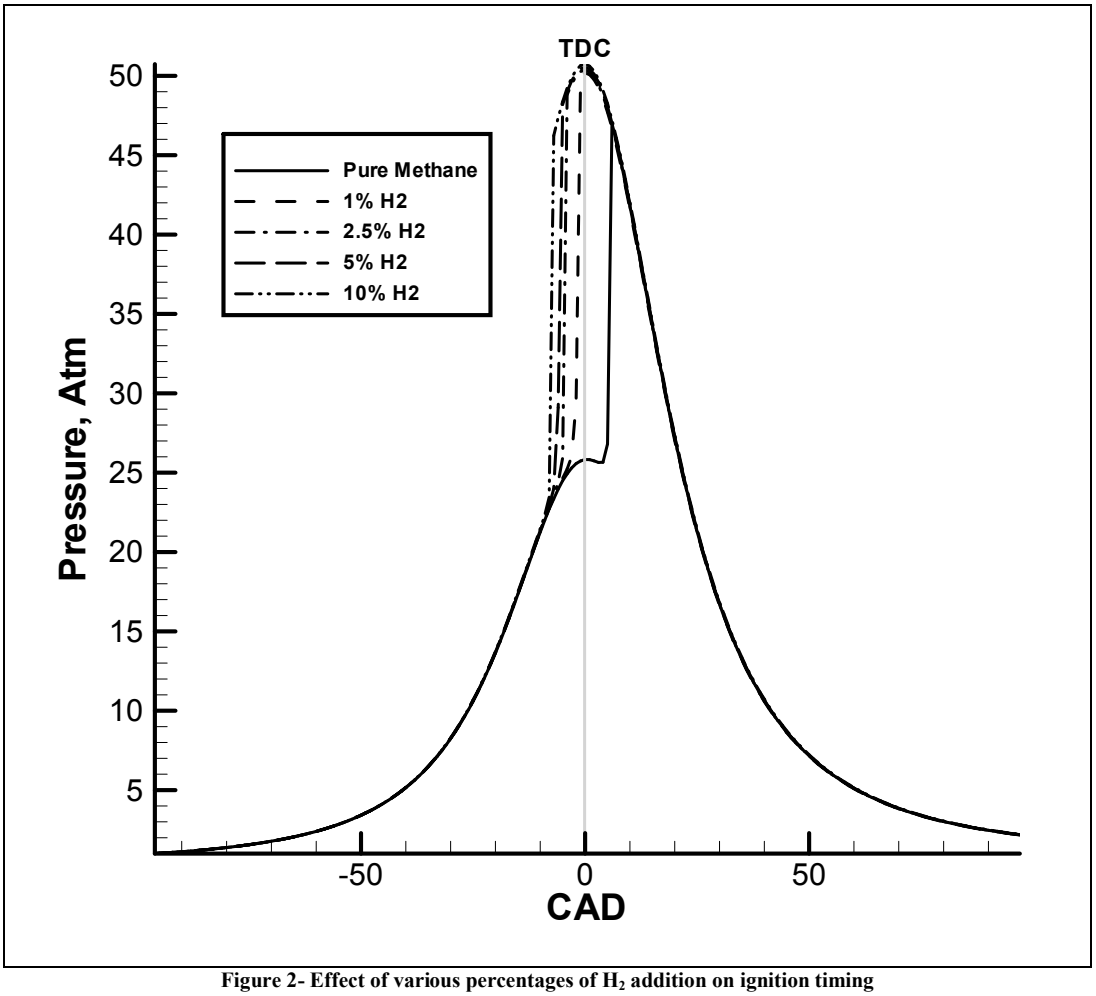


**Figure 2- Effect of various percentages of $H_2$ addition on ignition timing**

The reason for the effectiveness of the additive $(H_2)$ can be explained by the help of Fig. 3. The concentrations of $H_2O_2$ and radicals $H$, $OH$ and $HO_2$ are shown in the form of mass fraction as a function of crank angle during the HCCI combustion. These radicals are the most important promoters for driving the combustion.

In the case of $H_2$ addition, each $H_2$ atom at relatively high temperature decomposes into two $H$ radicals, which is a relatively good promoter for ignition. The importance of hydrogen addition as an additive in the combustion of methane will be as a contributor of H atoms, which are expected to facilitate the auto-ignition of the methane by enhancing the chain branching as in the $H_2/O_2$ reaction $(H + O_2 \rightarrow OH + O)$. As it can be seen, as amount of $H$ radical is decreased, simultaneously, the amount of $OH$ radicals is increased. This would advance the timing of the main heat release, translating into lower intake temperature required for stable auto-ignition of natural gas, especially at moderate compression ratios.

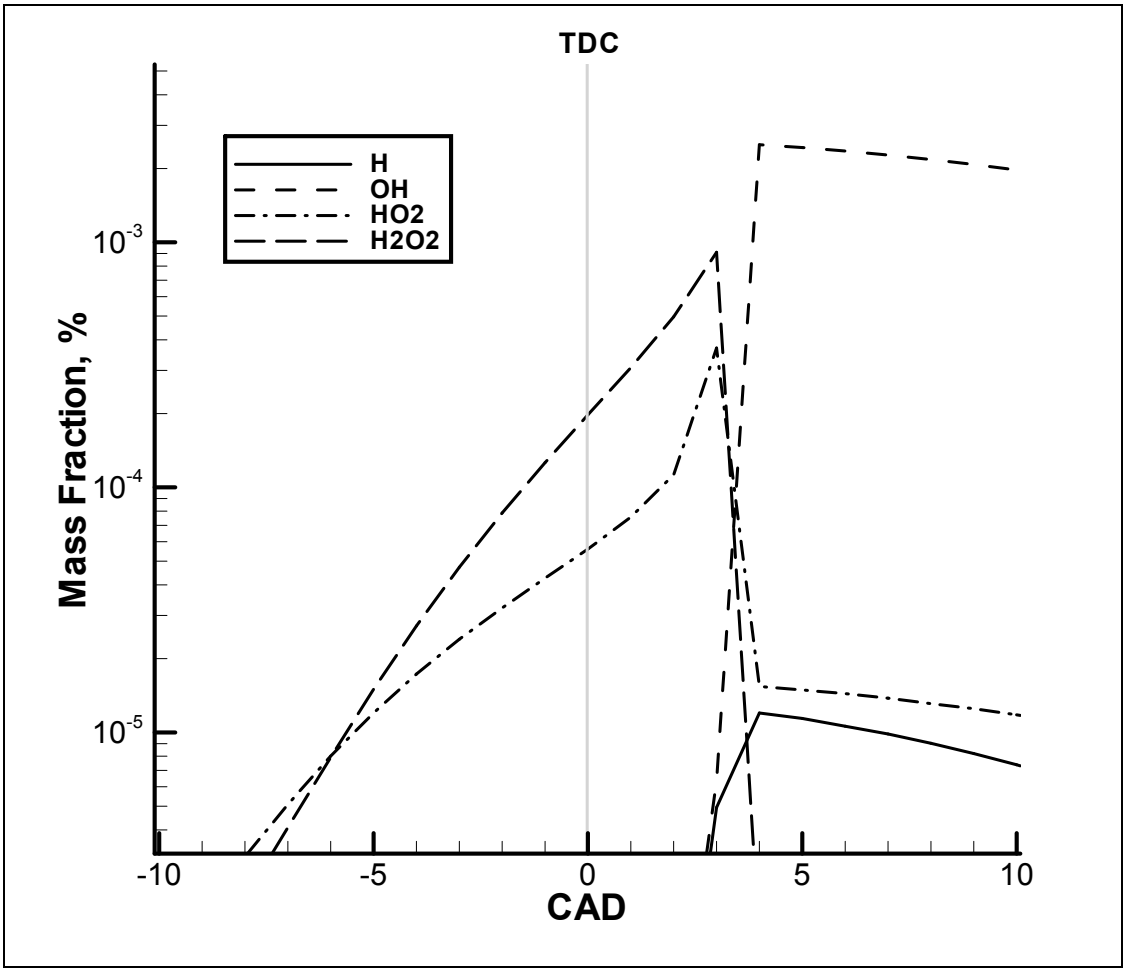


**Figure 3- Mass fraction of $H_2O_2$ and radicals H, OH, and $HO_2$ as a function of crank angle for 24% $H_2$ addition in order to achieve a near TDC ignition timing (T=450 K)**

The effect of engine speed on the required mass fraction of $H_2$ for near TDC ignition timing is investigated. The related profile is shown in Fig. 4. In this case the intake temperature and intake pressure are fixed at 510 K and 1 atm, respectively. The equivalence ratio is also fixed at 0.4 and the speed varies from 800 to 1800 rpm. The required mass fraction of additive for the near TDC ignition timing increases linearly with the increase of engine speed. When the engine speed is increased, the available reaction time for achieving the combustion is decreased. Hence, in order to achieve to the near TDC ignition timing, the amount of the additives must be increased. It can be seen that only the small amounts of $H_2$ is required.

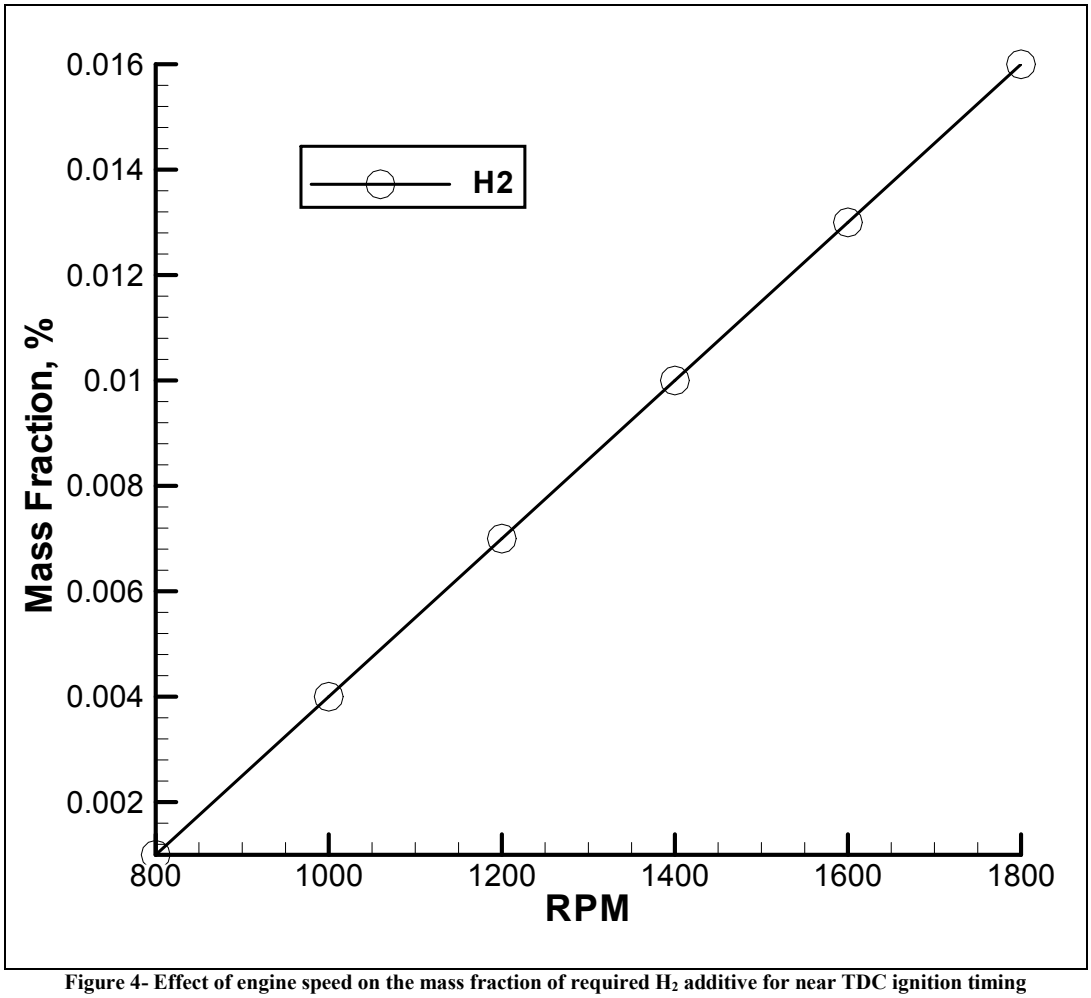


**Figure 4- Effect of engine speed on the mass fraction of required $H_2$ additive for near TDC ignition timing**

In next step the effect of equivalence ratio on the required mass fraction of each additive in order to achieve the near TDC ignition timing is examined. In this step the intake temperature and pressure are fixed at 510 K and 1 atm, respectively. The equivalence ratio is varied from 0.15 to .50 at the constant engine speed of 1000 rpm. The effect of equivalence ratio on the required mass fraction of $H_2$ addition in order to achieve the near TDC ignition timing is shown in Fig. 5. It is evident that with increasing the equivalence ratio, the increased fuel concentrations enhance the radical generation and results in a less amount of additive required for near TDC ignition timing. As it can be seen the required mass fractions of $H_2$ is very low.

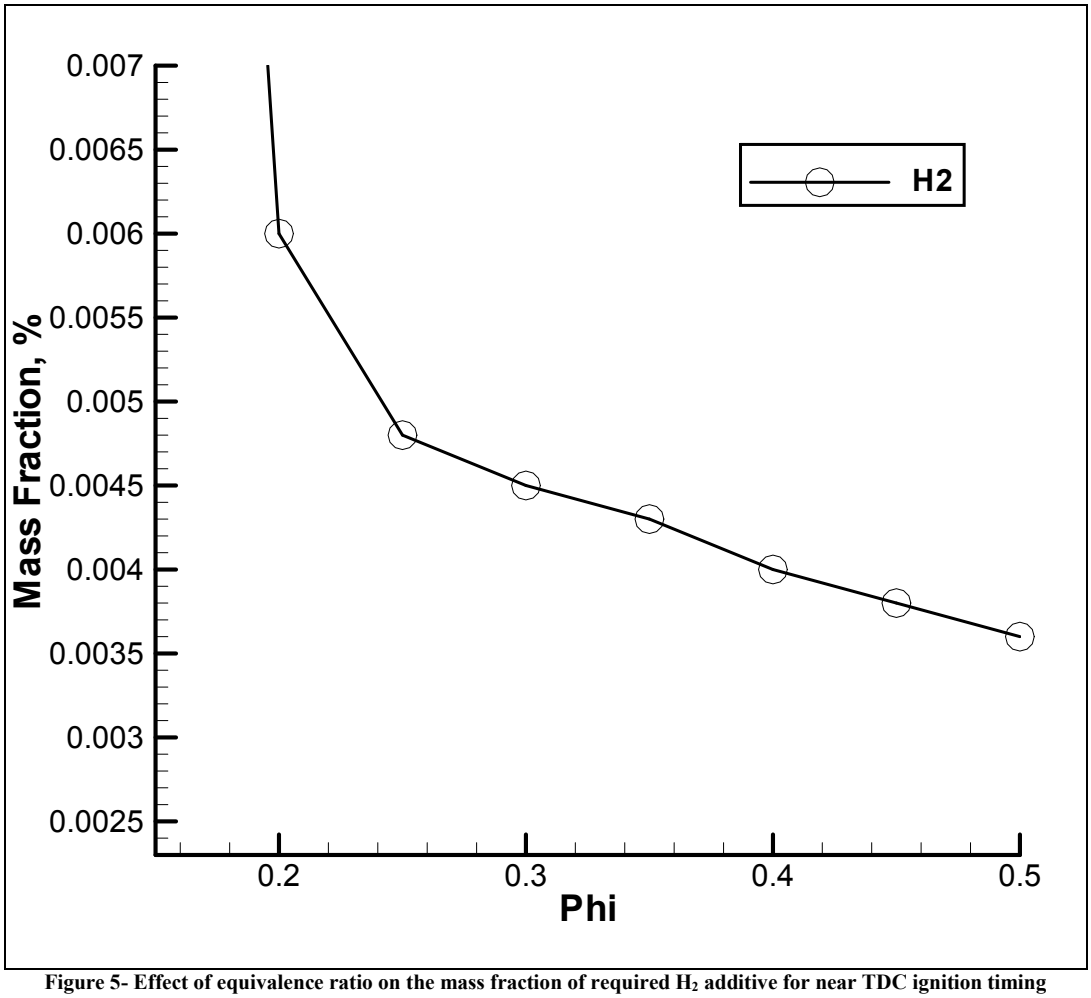


**Figure 5- Effect of equivalence ratio on the mass fraction of required $H_2$ additive for near TDC ignition timing**

In order to have the HCCI combustion in the lower intake temperature, the computations were conducted in order to reach the near TDC ignition timing with increased mass fraction of $H_2$ addition. The temperature decreased to 450K and the pressure and equivalence ratio were fixed at 1 atm and 0.4, respectively. The engine speed was also fixed at 1000 rpm. The minimum mass fractions required for starting the combustion at the reduced temperature of 450 K were calculated. The pressure traces for $H_2$ addition is shown in Fig. 6. It can be seen that the 24% mass fraction addition of $H_2$ is required in order to reach to the near TDC combustion.

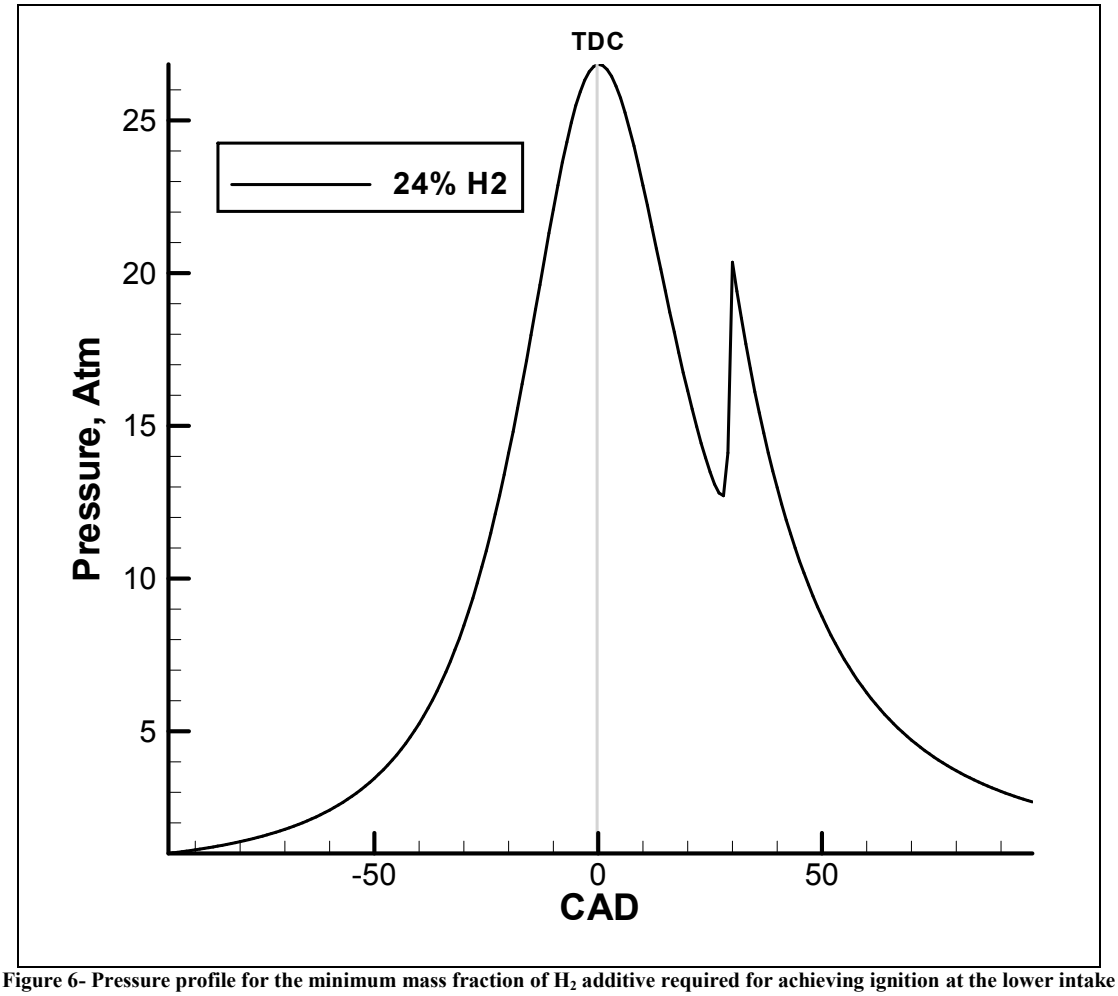


**Figure 6- Pressure profile for the minimum mass fraction of $H_2$ additive required for achieving ignition at the lower intake temperature (450 K)**

Finally the computations were conducted in order to evaluate the effect of different mass fraction of each additive at 450 K. The results of adding different mass fractions of each additive are shown in Fig. 7.

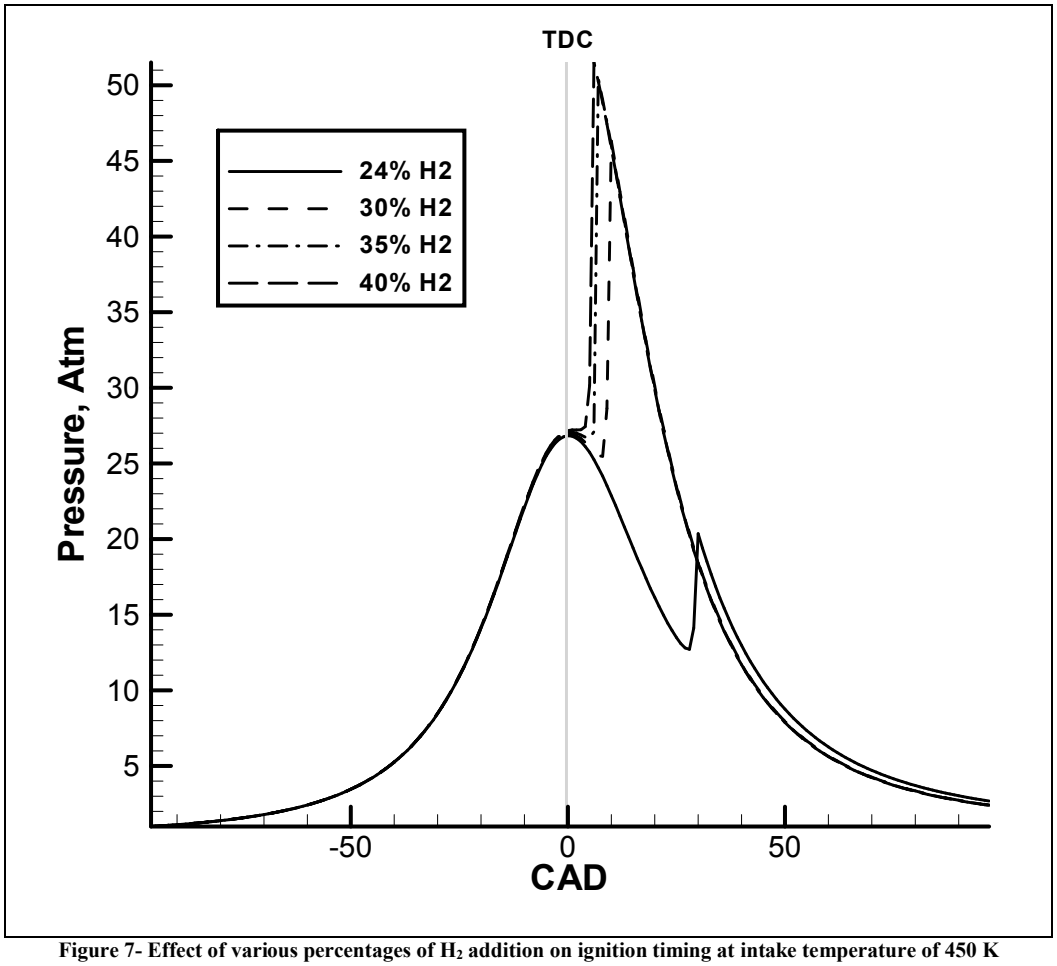


**Figure 7- Effect of various percentages of $H_2$ addition on ignition timing at intake temperature of 450 K**

## 4-Conclusion

The effect of addition of $H_2$ on the ignition timing of the Methane fueled HCCI engine, were studied numerically. The simulation has been conducted with the single zone zero-dimensional code in the CHEMKIN software. The GRI 3.0 chemical kinetics code that describes the natural gas kinetics has been used in this code. The variable volume with considering engine piston motion formulas was simulated in order to study the ignition of the Methane-fueled HCCI engine. The intake temperature and pressure were fixed at 510 K and 1 atm, respectively. The equivalence ratio was also fixed at 0.4. The conclusions of studies are as follow:

- The additives-free mixture did not ignite for the temperatures less than 510 K. It was found that addition small mass fraction of $H_2$ was effective in advancing the start of ignition timing as compared with the condition with no additive.
- It was found that with increasing the amount of $H_2$ additive, the start of ignition timing occurred earlier and the peak pressure was increased.
- It was obvious that the mass fraction of additive required to achieve a near TDC ignition timing increases linearly with the increase in the engine speed while decreases with the increase in the equivalence ratio.
- It can be seen that in order to reach the near TDC ignition timing, a mass fraction of 1% of $H_2$ is required.
- In order to achieve the near TDC ignition timing at lower intake temperature (450 K) the addition of even 24% by volume of $H_2$ could ignite a mixture.
- It is evident that reach the near TDC ignition timing at intake temperature of 450 K, a mass fraction of 40% of $H_2$ is required.

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