The effect of operational conditions on the ignition timing in the methane-fueled HCCI engine

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Abstract

Engine with the homogeneous charge compression ignition, HCCI, offers a number of benefits over conventional SI and CI, such as much lower NO_x emission and particulate matter emission. In this paper, the effects of intake temperature and pressure, equivalence ratio, engine speed and compression ratio on the auto ignition of the natural-gas HCCI engine have been investigated. 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 increasing the intake temperature and pressure would result in advance ignition and high peak temperature. It was also found that addition a small percent of Ethan and increasing the equivalence ratio would result in advance ignition, in contrast, increasing the equivalence ratio and engine speed retarded the ignition timing.

Keywords: Homogeneous Charge Compression Ignition (HCCI)-Chemical Kinetics-Auto ignition-Methane-fuel

1-Introduction

Homogeneous Charge Compression Ignition (HCCI) engine is currently under widespread investigation due to its high thermal efficiency close to that of diesel engines and low emissions of NO_x and particulate matter emissions. The first efforts to characterize HCCI combustion were done on two stroke engines [1, 2]. The primary reasons were to reduce unburned hydrocarbon (UHC) emissions at part load and to decrease fuel consumption by stabilizing the combustion of diluted mixtures. Based on the previous work in two-stroke engines, Najt and Foster extended the work to four-stroke engines and attempted to gain more comprehension on the underlying physics of HCCI combustion [3]. Thring further extended the work of Najt and Foster by examining the performance of an HCCI engine operated with a fully-blended gasoline [4]. Since then, a lot of research effort has been put on understanding HCCI combustion and how to control it. The HCCI engine can be operated under an ultra lean fuel condition. In addition, HCCI engines have been shown to operate with a range of fuels, i.e., gasoline, natural gas (NG), ethanol [5–7]. Unlike diesel combustion, where in-cylinder turbulence for flame diffusion is of great importance, or gasoline engine combustion where the mixture is ignited by spark and it is followed by the flame front propagation, HCCI combustion is ignited by the compression from the piston motion, so the fuel chemical kinetics plays a dominate role during the whole combustion process [6,7]. It is widely accepted that HCCI combustion is dominated by chemical kinetics of hydrocarbon oxidation chemistry, which in turn depend on the charge composition and the pressure and temperature histories of the reactants during the compression process. This notion has been supported by spectroscopy experiments, which indicate that the order of radical formation in HCCI combustion corresponds to that of self-ignition instead of flame propagation [8]. And as the effect of turbulence is negligible, it was not considered in our model. Therefore, understanding the chemical reactions is necessary to control the auto-ignition and combustion. Recent experimental [9] and modeling [10–12] efforts have also supported this idea. With rapid growth of the HCCI engine research, the study on chemical kinetics mechanism of many compounds becomes very active. In this study the effect of operational parameters on the ignition timing of the Methane fueled HCCI engine will be investigated.

2-Computational Model

A zero-dimensional model with an assumption of an adiabatic system is adopted. It is assumed that there is no heat transfer between the charge and the cylinder walls and that the pressure, temperature and concentrations

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of chemical species are all uniform in the cylinder. According to high speed of combustion in these types of engines, there is a small time for heat transferring between the cylinder and the outer environment, thus the assumption of adiabatic chamber does have a considerable effect on the results. 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. The SENKIN detailed chemical kinetics code from CHEMKIN 4.1 combustion package, which calculates the time evolution of the homogeneous reacting gas mixture in the combustion chamber, was used in the simulation [13]. SENKIN uses the differential algebraic sensitivity analysis code (DASAC) software to solve both the nonlinear ordinary differential equations that describe the temperature and species mass fractions and a set of linear differential equations that describe the first-order sensitivity coefficients of temperature and species composition with respect to the individual reaction rates [14]. The systems of ordinary differential equations that describe the physical problem are of the general form

$$\frac{dZ}{dt} = F(Z, t, a) \tag{1}$$

Where, in our case, $Z = (T, Y1, Y2, ..., YK)^T$ is the vector of temperature and mass fractions.

In early versions of SENKIN, the parameter vector a represented the pre-exponential constants a_i for each of the elementary reactions, as in Eq. (1). However, since CHEMKIN-II added rate formulations for pressure dependent reactions, it was necessary to include an extra parameter in the rate expression to allow perturbation of the rate. This extra parameter is normally one $(a_i = 1)$, except when DASAC perturbs it in computing the sensitivity solution. The first-order sensitivity coefficient matrix is defined as:

$$w_{i,j} = \frac{\partial Z_j}{\partial a_i} \tag{2}$$

Where the indices j and i refer to the dependent variables and reactions, respectively.

A positive percent change indicates a longer ignition delay and a decreased overall reaction rate, and a negative change indicates an increased overall reactivity of the system.

The natural-gas chemistry was described by the GRI-3.0 mechanism that considers 53 species and 325 reactions and used in order to investigate the effect of the intake pressure, intake temperature, compression ratio, engine speed, and the equivalence ratio on the auto ignition timing [15]. A premixed charge at uniform temperature and pressure is compressed and expanded at a rate that depends on the engine speed and geometry. The piston motion in the CHEMKIN software is defined with the following formula [16]:

$$\frac{V}{V_c} = 1 + \frac{1}{2}(r_c - 1)[R + 1 - \cos\theta - (R^2 - \sin^2\theta)^{\frac{1}{2}}] \tag{3}$$

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 θ is the crank angle. A transition from time to crank angle and vise versa could be made as:

$$t = \frac{\theta}{6N} \tag{4}$$

Where N is the engine speed in rpm.

The general form of the fundamental chemical reactions of the used mechanism is like as below:

$$\sum_{k=1}^{K} \upsilon'_{kj}\Gamma_k \leftrightarrow \sum_{k=1}^{K} \upsilon''_{kj}\Gamma_k, \quad j = 1..J \tag{5}$$

In order to solve the mass conservation equation the production rate of kth species is required, which can be calcualted with the following formula:
EQ2

$$\overset{\&}{\omega}_k = \sum_{j=1}^{J} \upsilon_{kj}q_j, \quad \upsilon_{kj} = \upsilon''_{kj} - \upsilon'_{kj} \tag{6}$$

The progression rate of reaction number j^{th} (q_j) is calculated from the following formula:

$$q_j = [M]_j \left(k_{fj} \prod_{k=1}^{K} C_k^{\upsilon'_{kj}} - k_{bj} \prod_{k=1}^{K} C_k^{\upsilon''_{kj}} \right) \tag{7}$$

If the third specis does not exist in a reaction, the amount of $[M]_j$ will be equall to one, else it can be calculated from the followinfg frormula:

$$[M]_j = \sum_{k=1}^{K} \alpha_{kj} C_k \tag{8}$$

Amounts of α_{kj} in the used equation, is available for the reactions with presence of third species. For calculating the q_j, the amounts of k_{fj} and k_{bj} are required. Calculating the k_{fj} depends on the type of equation and in equation with no pressure dependency it can be calculated from the Arrhenius equation as follow:

$$k_{fj} = A_j T^{\beta_j} \exp\left(\frac{-E_j}{R_c T} \right) \tag{9}$$

The amounts of A_j, β_j and E_j for all reactions are available. For pressure dependent reactions, the trend is more sophisticated.

$$P_{rj} = \frac{k_{0j} [M]_j}{k_{\infty j}} \tag{10}$$

$$k_{fj} = k_{\infty j} \left(\frac{Pr_j}{1 + Pr_j} \right) F \tag{11}$$

k_{0j} and $k_{\infty j}$ are calculated from equation 9 and their coefficients are calculated from the GRI mechanism. The amount of Fj for each reaction can be calculated with Lindemann, Troeh or Stewart forms. In the GRI mechanism just two first forms are used. In Lindeman, the amount of F_j is equal to 1. But in the Troeh form, the F_j is assumed to be variable and calculated from the complicated equation[13]. With calculating the amount of kfj, the amount of k_{bj}, can be calcualted easily. After calculating the dimensionless terms of $\frac{H_K}{R_u T}$ and $\frac{S_K}{R_u}$, the variation of entropy and anthalpy are calculated for each reaction.

$$\frac{\Delta S_j}{R_u} = \sum_{k=1}^{K} \upsilon_{kj} \frac{S_k}{R_u} \tag{12}$$

$$\frac{\Delta H_j}{R_u T} = \sum_{k=1}^{K} \upsilon_{kj} \frac{H_k}{R_u T} \tag{13}$$

Then the pressure balance coefficient for each reaction is calculated.

$$K_{pj} = \exp\left(\frac{\Delta S_j}{R_u} - \frac{\Delta H_j}{R_u T} \right) \tag{14}$$

Balance coefficient in term of molar concentration, calculated from the below equation

$$K_{cj} = K_{pj} \left(\frac{P_{atm}}{R_u T} \right)^{\sum \upsilon_{kj}} \tag{15}$$

Finally the retrogression coefficient of the reaction number j[th] calculated from the following equation.

$$k_{bj} = \frac{k_{fj}}{K_{Cj}} \tag{16}$$

In order to solve the mentioned equation the DVODE [17]subroutine was used.

In this study the 6-cylinder diesel engine geometry was used. 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

In order to study the effect of the operational conditions on the ignition timing of the Methane fueled HCCI engine, the engine with the specification mentioned in table 1 is used. The calculations are carried out in the nominal conditions as: intake temperature of 510K, intake pressure of 1 atm, and the equivalence ratio of 0.4. The effect of varying different parameters on the ignition timing were investigated and the results are as follow.

3-1-Effect of intake temperature variation:

HCCI combustion is predominated by chemical reaction, and then the intake charge temperature becomes the most important factor that effects the HCCI ignition. In this part of our study the intake temperature varies from 490 K to 530 K and its effect on the ignition timing will be investigated. As it is obvious inn Fig. 1, methane does ignite for an intake manifold temperature of 490 K, consistent with previous studies [19, 20]. With increasing the inlet temperature the ignition timing will be advanced and as it can be seen in the inlet temperature of 530 K the near TDC ignition timing will occur. An increase in the inlet temperature reduces trapped mass and volumetric efficiency, which in turns adversely affects torque and power output. Advanced ignition, which increases compression effort, combined with reduced volumetric efficiencies leads to a reduction in net indicated thermal efficiency. The best combustion timing depends on a variety of factors and likely varies depending on the operating conditions.
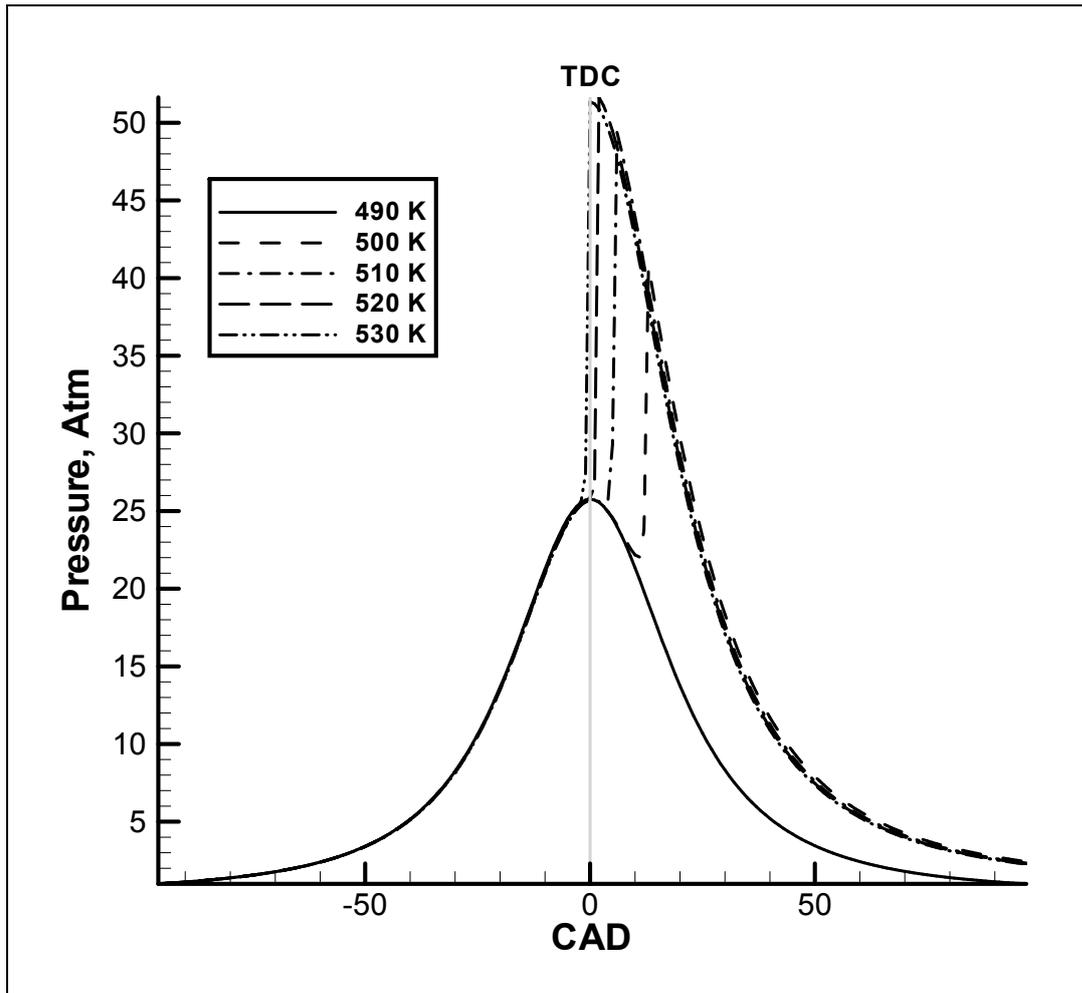
Figure 1-The pressure trace for variation of inlet temperature

3-2-Effect of intake pressure variation:

In this part of our study the inlet temperature and equivalence ratio will be fixed at 510 K and 0.4, respectively. The inlet pressure varies from 0.8 atm to 2.5 atm and its effect on the ignition timing will be investigated. As it can be seen in Fig. 2, the very poor and late combustion occurs at 0.8 atm and with increasing the inlet pressure, the ignition timing is advanced and also the peak pressure is increased. The near TDC ignition timing occurs at inlet pressures between 1.5 atm to 2 atm.
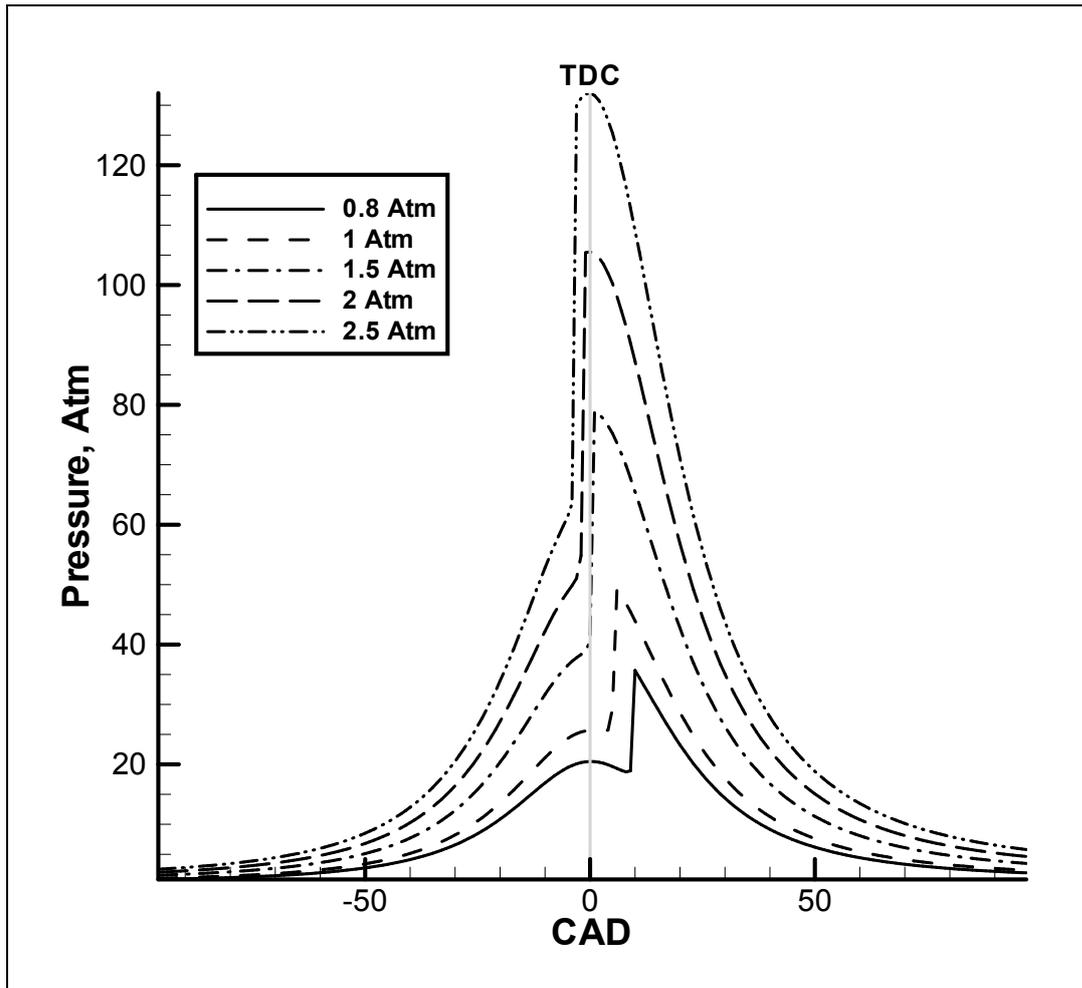
Figure 2-The pressure trace for variation of intake pressure

3-3-Effect of engine speed variation:

In this part, the inlet temperature and inlet pressure will be fixed at 510 K and 1 atm, respectively. The engine speed varies from 700 RPM to 1500 RPM and its effect on the ignition timing will be investigated. According to Fig. 3, as the engine speed is increased, the start of ignition is retarded. At engine speed of 1500 RPM the mixture does not ignite anymore. With increasing the engine speed, the available time for igniting the mixture is decreased and due to the fact that HCCI combustion is kinetic dependant combustion, the mixture will not have enough time to reach to the ignition condition and because of that at higher engine speed the mixture does not ignite. As it is evident in Fig. 3, the near TDC combustion occurs at the engine speed between 700 RPM and 900 RPM.
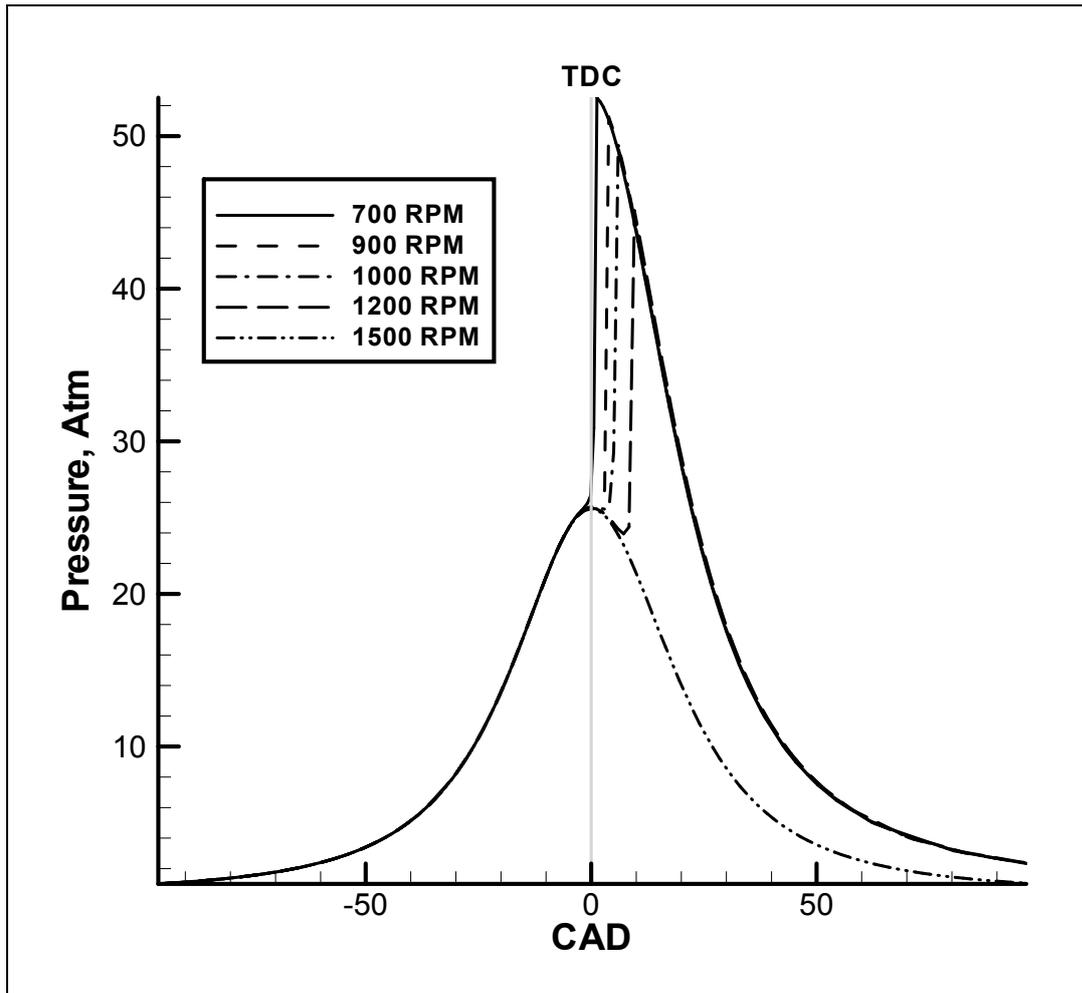
Figure 3-The pressure trace for variation of engine speed

3-4-Effect of compression ratio variation:

In this part, the inlet temperature and inlet pressure will be fixed at 510 K and 1 atm, respectively. The compression ratio of engine varies from 16.5 to 19 and its effect on the ignition timing will be investigated. As it is evident in Fig. 4, in compression ratio of 16.5, the mixture does not ignite. With increasing the compression ratio of engine, the start of ignition is advanced. The near TDC ignition timing occurs in compression ratio between 18 and 19.
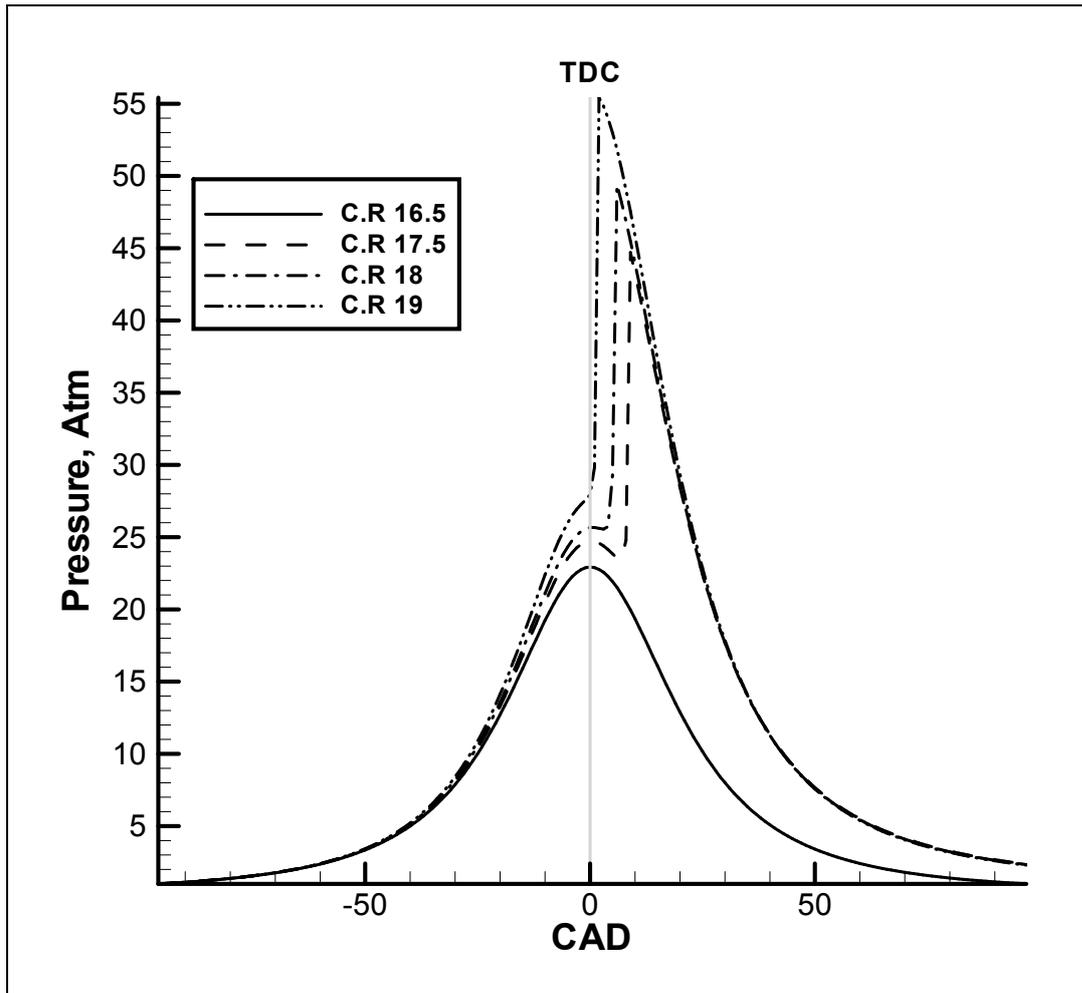
Figure 4-The pressure trace for variation of engine compression ratio

3-5-Effect of equivalence ratio variation:

In this part, the inlet temperature and inlet pressure will be fixed at 510 K and 1 atm, respectively. The equivalence ratio of mixture varies from 0.3 to 0.6 and its effect on the ignition timing will be investigated. It can be seen in Fig. 5 that the mixture even ignites in equivalence ratio of 0.3 and in compare with commercial compression ignition engines; this mixture is by far leaner. Using the lean mixture has a big advantage that the specific heat of the mixture decreases and hence the peak temperature decreases [21]. Further increase in equivalence ratio leads to the more ignition delay.

In Fig. 6 and the mass fraction of H radicals are shown for two different cases. Calculations carried out for intake temperatures of 490 K and 510 K. As it is evident in Fig. 6, the mass fraction of H radicals does not change in the case that the inlet temperature is 490 K and remain at the value of zero, but in the case that the inlet temperature is 510 K, as the H radicals have the significant role in combustion reactions, the mass fraction of the mentioned radicals has a sudden increase near the TDC and after that gradually decreases to reach the amount of zero.

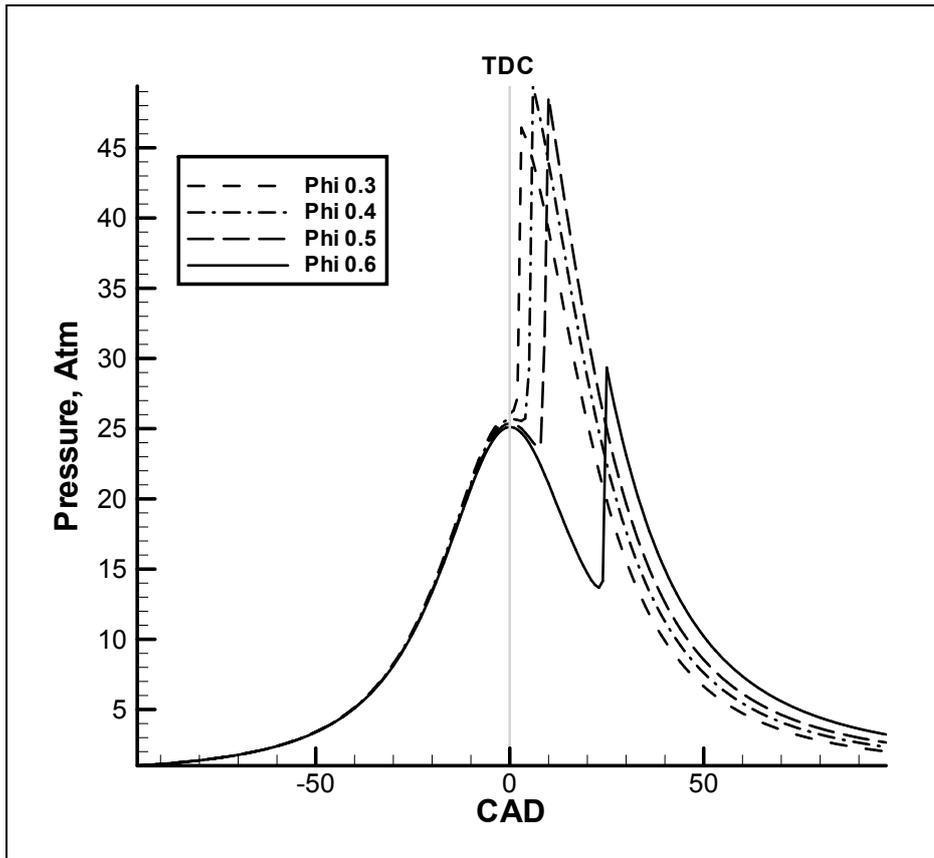Such a trend also can be seen in Fig. 7 for the OH radicals.

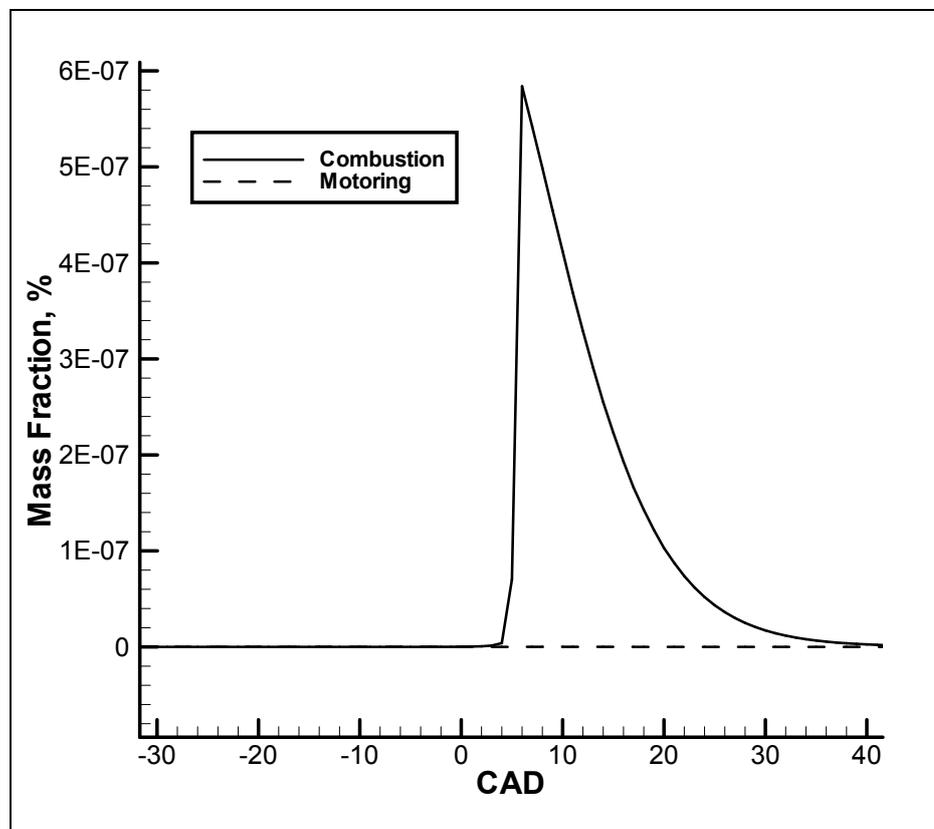**Figure 5-The pressure trace for variation of equivalence ratio**

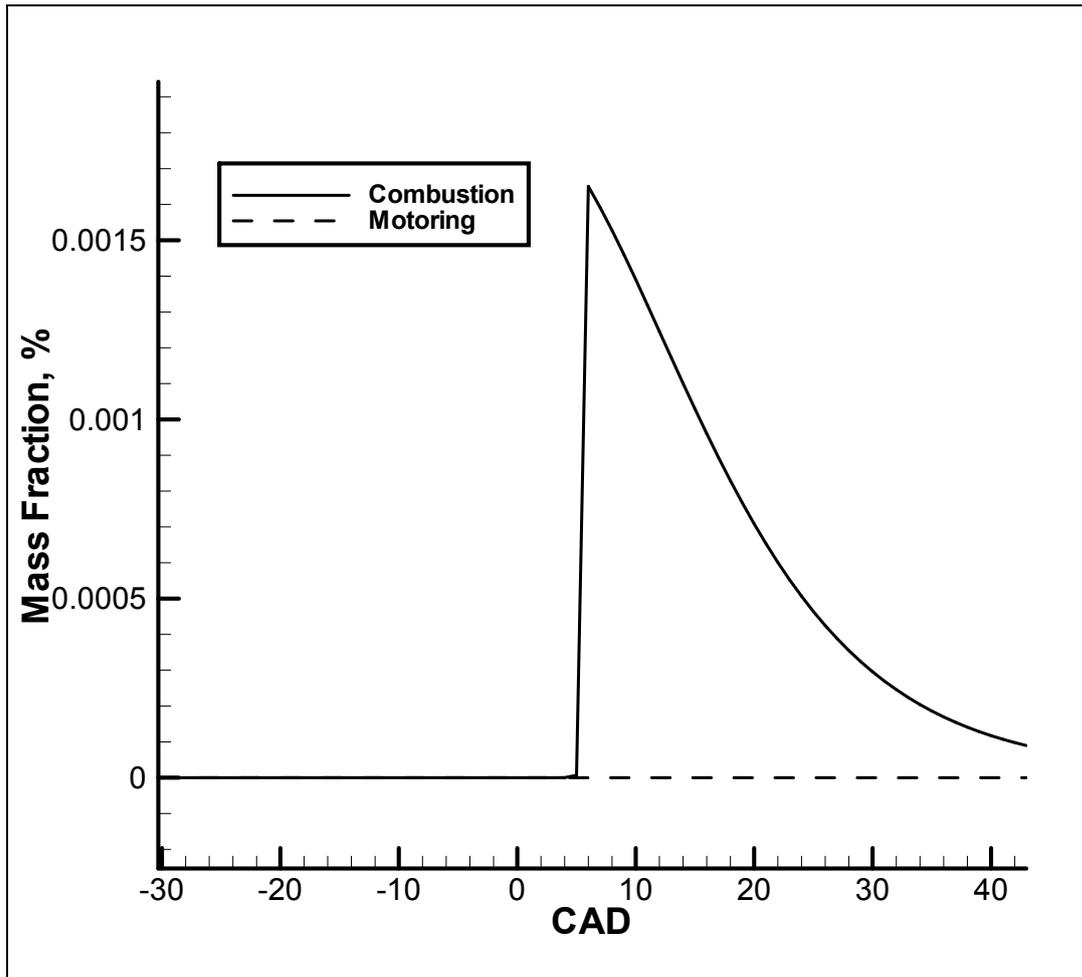**Figure 6-Mass fraction of H radicals for two different cases**

Figure 7- Mass fraction of H radicals for two different cases

3-6-Effect of fuel chemical composition:

In the similar operational condition, small percent of Ethane is added to the mixture. As it can be seen in Fig. 8, addition small mass fraction of Ethane to the mixture, advance the start of ignition considerably and it conforms to previous studies [22]. On the other hand, it increases the peak pressure of the combustion. Hence the amount of Ethane addition must be determined in order to give the near TDC start of ignition with the regulated peak pressure.
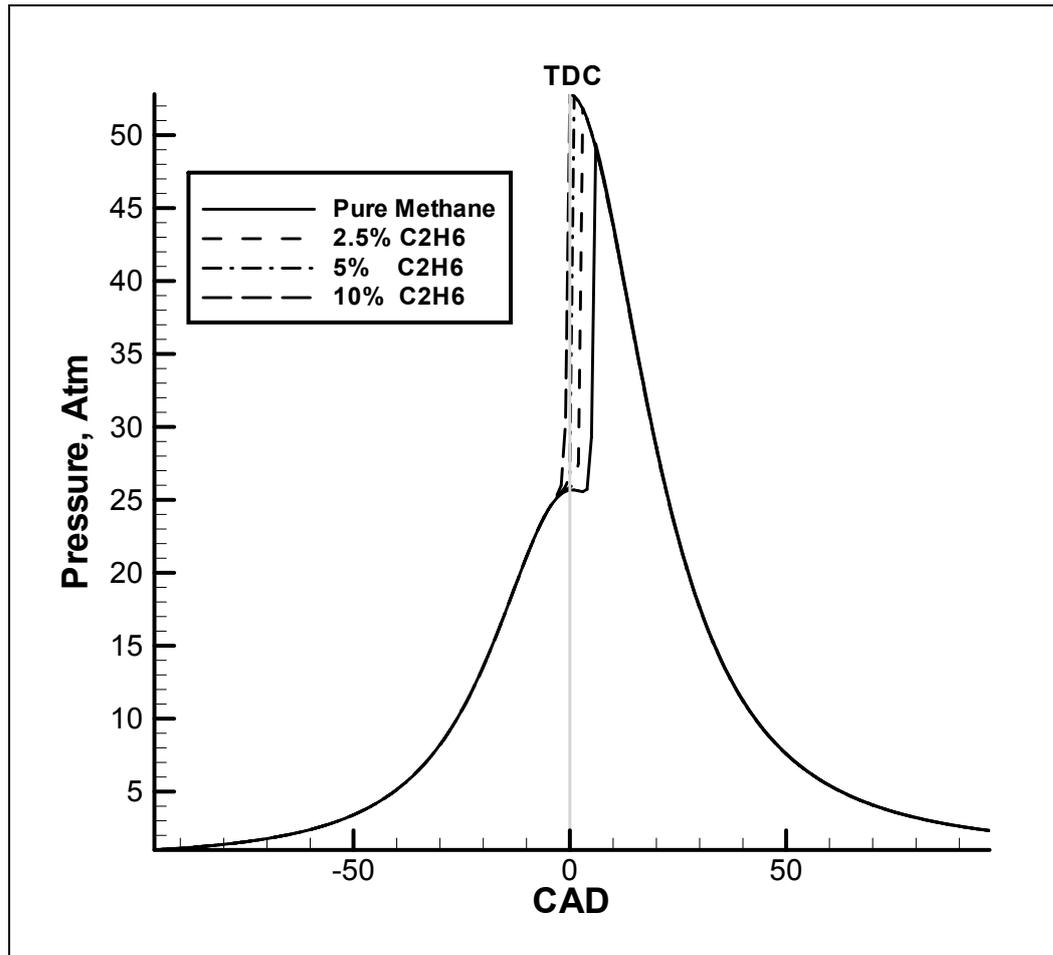
Figure 8-The pressure trace for addition of different mass fractionsEthane

4-Conclusion

The effect of operational condition on the ignition timing of the Methane fueled HCCI engine, were studied numerically. The simulation has been conducted with the adiabatic 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 effect of varying intake temperature, intake pressure, engine speed, compression ratio, and equivalence ratio were studied. Finally the effect of gas composition on the ignition timing was investigated. The conclusions of studies are as follow:

- Increasing the inlet temperature and pressure led to advanced start of ignition. And also the peak pressure increased incredibly for both cases, but the effect of increasing the temperature was more obvious. The sensitivity of the ignition timing to the inlet pressure is very low and especially in high pressure it does not have a significant effect on the ignition timing.

- It was found that increasing the engine speed and equivalence ratio would retard the ignition timing.

- It was found that increasing the compression ratio would result in advanced start of ignition and the peak pressure also increased incredibly.

- It was found that when there is no combustion in the chamber, the amount of H and OH radicals were equal to zero and had no distinct variation, but in the time that there was combustion in the engine, the amount o H and OH radicals increased suddenly near the TDC and after that decreased gradually.

- Addition small amount of C2H6 to the mixture at inlet temperature of 510 K, resulted in a very advanced start of ignition and its effect was evident.

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