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INVESTIGATION OF VARIATION IN CYLINDER PARAMETERS IN A SPARK IGNITION NATURAL GAS ENGINE WITH NATURAL GAS-HYDROGEN BLENDS

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ABSTRACT

This study presents the numerical simulations of combustion of methane-hydrogen blends (100%CH₄, 10% H₂ - 90%CH₄, 20%H₂ - 80%CH₄ and 30%H₂ - 70%CH₄) through a cylinder. The numerical calculations were performed using the finite volume CFD code FLUENT with the standart k-ε model, for which the compression ratio and the nominal speed are 10 and 2000 rpm, respectively. Excessive air ratios were selected as 0.8, 1.0, 1.2 and 1.4. The spark timings were started 30° BTDC. The results of the combustion process were investigated as a function of crank angle. Calculated cylinder pressure data was compared with experimental for the verification of the combustion model, this investigate reveals that the combustion model used shows encouraging results. The maximum cylinder pressures and temperatures were obtained as a consequence of rich mixture. When the excessive air ratio increased, peak pressure values are decreased.

Keywords: Methane, Hydrogen, Spark Ignition Engine, Modeling, Emissions

INTRODUCTION

The energy system today is dominated by fossil fuels, which are abundant and relatively inexpensive. Burning of the fossil fuels generates waste materials, mainly emissions to the atmosphere in the form of combustion fuel gases and dust, as well as some ash and/or clinker. These waste materials have hazardous effects on the environment, some of them locally, others with more widespread or even global impact [1]. Natural gas (NG) is an extremely important source of energy for reducing pollution and maintaining a clean and healthy environment. In addition to being a domestically abundant and secure source of energy, the use of NG also offers a number of environmental benefits over other sources of energy, particularly other fossil fuels [2]. Natural gas is composed primarily of methane which dominates its emission characteristics. Methane mixes readily with air and has a high octane rating which makes it a very good spark-ignition engine fuel [3].

NOMENCLATURE

A area
A empirical constant (4.0)
AFR air/fuel ratio
ATDC After top dead center
B empirical constant (0.5)
BTDC Before top dead center
BDC Bottom dead center
CA Crank angle
C_{j,r} molar concentration of each reactant and product species j
C_μ model constant for RNG-k-ε model
C_{1ε} coefficient in RNG-k-ε model
C_{2ε} coefficient in RNG-k-ε model
CFD Computational Fluid Dynamics
EAR Excessive air ratio
G_k the production of turbulent kinetic energy
k turbulent kinetic energy
MBT maximum brake torque
NG Natural gas
Nr number of chemical species in reaction r
 $\eta_{j,r}^i$ forward rate exponent for each reactant and product species j
 $\eta_{j,r}^u$ backward rate exponent for each reactant and product species j
P pressure
q^{''} heat flux per unit area
RPM revulation per minute
R_{i,l} mass rate of creation or depletion by chemical reaction
R_{i',k} reaction rate
RNG renormalization group
SI Spark ignition
ST spark timing
T temperature
TDC top dead center
v^l stoichiometric coefficient for reactant
v^u stoichiometric coefficient for product
V volume
Y_P is the mass fraction of any product species, P
Y_R is the mass fraction of a particular reactant, R,

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Greek symbols

α	inverse effective Prandtl number
χ	additional term in the ε equation
ε	turbulent energy dissipation rate
ϕ	equivalence ratio
λ	excessive air ratio
μ	dynamic viscosity
ρ	density

One of the problems with petroleum is the emission of pollutants, such as CO_2 , NO_x , CO and hydrocarbons (HC). Much greater amounts of coal are known to exist but conventional coal burning technology is much more polluting than most other fuels, particularly in terms of the greenhouse gas emissions per unit of useful energy released [1]. In order to decrease these pollutions, alternative fuels are being considered such as methane, hydrogen and mixtures of hydrogen and methane.

A major difficulty in the operation of engines whether of the spark ignition or compression ignition types on lean mixtures of methane and air is the associated low flame propagation velocity. Some improvement to the burning rate in spark ignition engines is usually obtained through measures such as the employment of optimum spark timing, improved chamber design and increased turbulence. The extent of increase in the level of turbulence in engines is usually limited and there are penalties associated with the use of excessive turbulence that includes excessive heat transfer and higher NO_x emissions in optimum chamber geometry [4].

Sitthiracha and et. al., have been developed Mathematical model of spark ignition engine using cylinder-by-cylinder model approach in order to predict the performances; torque and power. The method is based on ideal Otto cycle and modified by equations which affect the performances. The model consists of set of tuning parameters such as engine physical geometries, ignition advanced, air/fuel ratio, etc. They are also developed under Matlab/Simulink. Their results from simulation are verified with the data from commercial engines [5].

Shudo and et. al., have been analyzed characteristics of combustion and emissions in a methane direct injection stratified charge engine premixed with hydrogen lean mixture [6]. Their results displayed the combustion system achieved a higher thermal efficiency due to higher flame propagation velocity and lower exhaust emissions. An increase in the amount of premixed hydrogen stabilizes the combustion to reduce HC and CO exhaust emission, and increases the degree of constant volume combustion and NO_x exhaust emission. The increase in NO_x emission can be maintained at a lower level with retarded ignition timing without deteriorating the improved thermal efficiency.

Papagiannakis and Hountalas have been concerned, with an experimental investigation of the characteristics of dual fuel operation when liquid diesel is partially replaced with natural gas under ambient intake temperature in a DI diesel engine. Results were given revealing the effect of liquid fuel percentage replacement by natural gas on engine performance and emissions [7]. As far as pollutant emissions are

Subscripts

eff	effective
i, j	indices of tensor notation
i', j'	species no
mwa	mass-weighted average
P	product species no
R	reactant species no

concerned, the use of gaseous fuel has a positive effect on NO emissions. The level of NO concentration under dual fuel operation is lower compared to the one under normal diesel operation. Under dual fuel operation, CO and HC emissions are generally higher in comparison with normal diesel operation. Their value increases with the gaseous fuel mass ratio and only at high engine load and high natural gas mass ratios a decrease was observed.

Akansu et al. [8, 9], Çeper et al. [10], and Kahraman et al. [11] examined the burning of methane-hydrogen mixtures in internal combustion engines. They found that methane-hydrogen mixtures helped decreasing exhaust emissions, such as HC, CO, CO_2 , and the engine efficiency could be increased under certain conditions

Abd Alla analyzed the preliminary simulation of a four stroke spark ignition engine. An arbitrary heat release formula was used to predict the cylinder pressure. This cylinder pressure was used to find the indicated work done. The heat transfer from the cylinder, friction and pumping losses also were taken into account to predict the brake mean effective pressure, brake thermal efficiency and brake specific fuel consumption. Most of the parameters that can affect the performance of four stroke spark ignition engines, such as equivalence ratio, spark timing, heat release rate, compression ratio, compression index and expansion index are studied. The use of a real combustion curve has a profound influence on the similarity of the pressure-volume profile to the one which is seen for the real engine. The modeling process is obviously getting closer to reality and is now worth pursuing as a design aid [12].

Ohyama studied on the combination of physical models of an advanced engine control system. Advanced engine control system was proposed to obtain sophisticated combustion control in ultra-lean combustion, including homogeneous compression-ignition and activated radical combustion with a light load and in stoichiometric mixture combustion with a full load. Physical models of intake, combustion and engine thermodynamics were incorporated, in which the effects of residual gas from prior cycles on intake air mass and combustion were taken into consideration. The combined control of compression ignition at a light load and spark ignition at full load for a high compression ratio engine was investigated using simulations. The control strategies of the variable valve timing and the intake pressure were clarified to keep auto-ignition at a low load and prevent knock at a full load [13].

Akansu et al. [14] numerically studied hydrogen-air combustion in a SI engine. They stated that hydrogen-air

mixture of calculated in-cylinder pressure indicated good agreement for excessive air ratios between 2 and 2.4.

Muk Cho and He studied natural gas as a review study. In their paper, the operating envelope, fuel economy, emissions, cycle-to-cycle variations in indicated mean effective pressure and strategies to achieve stable combustion of lean burn natural gas engines are highlighted. Stoichiometric natural gas engines are briefly reviewed. To keep the output power and torque of natural gas engines comparable to those of their gasoline or Diesel counterparts, high boost pressure should be used. High activity catalyst for methane oxidation and lean deNOx system or three way catalyst with precise air–fuel ratio control strategies should be developed to meet future stringent emission standards [15].

One of the major areas of development in the internal combustion engine is the development of computer simulations of various types of engines. Their economic value is in the reduction in time and costs for the development of new engines and their technical value is in the identification of areas that require specific attention as the design study evolves. Computer simulations of internal combustion engine cycles are desirable because of the aid they provide in design studies, in predicting trends, in serving as diagnostic tools, in giving more data than are normally obtainable from experiments, and in helping one to understand the complex processes that occur in the combustion chamber. In the present work, two-dimensional model was developed to simulate a 4-stroke cycle of a spark ignition engine fueled with methane-air mixture depending on crankshaft angle. In order to investigate the effect of spark timing and excessive air ratios on the combustion, the combustion of methane with air is examined at various ignition advance and excessive air ratios by using Fluent CFD code [16].

MATHEMATICAL MODEL

Cylinder Geometry

In this study, variations of temperature, pressure, emissions and turbulent rate of reactions in cylinder has been estimated. For this purpose, the combustion of methane-hydrogen mixtures in a cylinder has been considered. Spark timing ratio has been selected BTDC 30 CA, and excessive air ratio (λ) has been taken 0.8, 1, 1.2, and 1.4. The two-dimensional model and dimensions of this considered cylinder are shown in Figure 1. As apparent from this figure, the methane-hydrogen mixtures enters intake valve and burned gas goes out exhaust valve. Piston moves from TDC to BDC. Crank shaft speed is taken 2000 rpm. The main geometrical details of the engine are as given in Table 1.

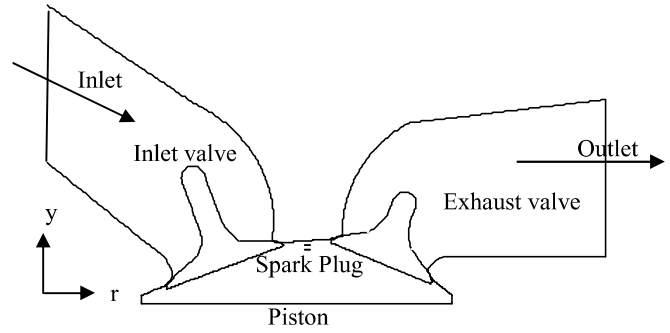


Figure 1 Two dimensional cylinder geometry.

Table 1 Engine specifications

Bore	80.6	mm
Stroke	88	mm
Compression Ratio	10:1	-
Exhaust valve opening	55	BBDC
Exhaust valve closing	50	ATDC
Intake valve opening	13	BTDC
Intake valve closing	47	ABDC
Intake valve radius	30	mm
Exhaust valve radius	28	mm

Mathematical model

Combustion takes place in the cylinder during the closed period and is that time in the engine cycle when all the valves are closed.

The models used for the numerical calculations are as follows:

- For the turbulent flow, the standart k-ε model [16].
- For the chemical species transport and reacting flow, the eddy-dissipation model and the eddy dissipation concept.

The assumptions made are as follows:

- The flow is steady, two-dimensional and compressible.
- The fuel-air mixture is assumed as ideal gas.
- Cylinder walls are constant temperature.

Two additional equations for the standart k-ε turbulence model: The turbulence kinetic energy, k, and the dissipation rate, ε, are determined using the following transport equations, respectively:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \rho \epsilon - Y_M + S_k \tag{1}$$

$$\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial x_i}(\rho \epsilon u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + C_{1\epsilon} \frac{\epsilon}{k} (G_k + C_{3\epsilon} G_b) - C_{2\epsilon} \rho \frac{\epsilon^2}{k} + S_\epsilon \tag{1}$$

In these equations, G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients, G_b is the generation of turbulence kinetic energy due to buoyancy, Y_M represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate, $C_{1\epsilon}$, $C_{2\epsilon}$ and $C_{3\epsilon}$ are constants. σ_k and σ_ϵ are the turbulent Prandtl numbers for k and ε, respectively. S_k and S_ϵ are user-defined source terms.

The Eddy Dissipation Model :

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The net rate of production of species i due to reaction r , $R_{i,r}$, is given by the smaller (i.e., limiting value) of the two expressions below:

$$R_{i^1,k} = v_{i^1,k}^1 M_{i^1} A \rho \frac{\varepsilon}{k} \frac{m_R}{v_{R,k}^1 M_R} \quad (2 \text{ a,b})$$

$$R_{i^1,k} = v_{i^1,k}^1 M_{i^1} A B \rho \frac{\varepsilon}{k} \frac{\sum_P m_P}{\sum_{j^1}^N v_{j^1,k}^1 M_{j^1}}$$

where Y_P is the mass fraction of any product species, P
 Y_R is the mass fraction of a particular reactant, R ,
 A is an empirical constant equal to 4.0
 B is an empirical constant equal to 0.5

In Equations 2a,b, the chemical reaction rate is governed by the large eddy mixing time scale [16]. Combustion proceeds whenever turbulence is present ($k/\varepsilon > 0$), and an ignition source is not required to initiate combustion. This is usually acceptable for non-premixed flames, but in premixed flames, the reactants will burn as soon as they enter the computational domain, upstream of the flame stabilizer. To remedy this, FLUENT provides the finite-rate/eddy dissipation model, where both the Arrhenius (Equation 4), and eddy-dissipation (Equations 2a,b) reaction rates are calculated. The net reaction rate is taken as the minimum of these two rates. In practice, the Arrhenius rate acts as a kinetic "switch", preventing reaction before the flame holder. Once the flame is ignited, the eddy-dissipation rate is generally smaller than the Arrhenius rate, and reactions are mixing-limited.

The molar rate of creation/destruction of species i in reaction r ($\widehat{R}_{i,r}$, Equation 4) is given by

$$\widehat{R}_{i^1,k} = \Gamma(v_{i^1,r}'' - v_{i^1,r}') (k_{f,r} \prod_{j=1}^{N_r} [C_{j,r}]^{\eta_{j,r}'} - k_{b,r} \prod_{j=1}^{N_r} [C_{j,r}]^{\eta_{j,r}''}) \quad (3)$$

where

N_r number of chemical species in reaction r

$C_{j,r}$ molar concentration of each reactant and product species j in reaction r (kgmol/m³)

$\eta_{j,r}^1$ forward rate exponent for each reactant and product species j in reaction r

$\eta_{j,r}^1$ backward rate exponent for each reactant and product species j in reaction r

The eddy dissipation concepts model;

The eddy-dissipation-concept (EDC) model is an extension of the eddy-dissipation model to include detailed chemical mechanisms in turbulent flows. It assumes that reaction occurs in small turbulent structures, called the fine scales. The volume fraction of the fine scales is modeled as:

$$\xi^* = C_\xi \left(\frac{\nu \varepsilon}{k^2} \right)^{3/4} \quad (4)$$

where ξ^* denotes fine scale quantities and C_ξ volume fraction constant (2.1377), ν kinematic viscosity

Species are assumed to react in the fine structures over a time scale

$$\tau^* = C_T \left(\frac{\nu}{\varepsilon} \right)^{1/2} \quad (5)$$

Where C_T is a time scale constant equal to 0.4082.

The thermal properties of mixture: The density is ideal gas, specific heat is mixing law, viscosity and thermal conductivity are assumed constant.

Boundary conditions:

At the intake valve; $u_i = U_y$ and $T = T_{in} = 300$ K,

$$l = 0.07 D_H, \quad k = \frac{3}{2} (IU_{ort})^2 \quad \text{and} \quad \varepsilon = C_\mu^{3/4} \frac{k^{3/2}}{l} \quad (6)$$

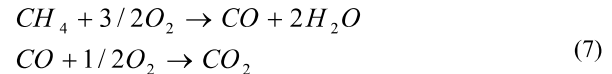
At the exhaust valve; Pressure outlet= atmospheric medium
 At the cylinder wall; $u_r = 0$, $u_y = 0$, $T = T_d = 360$ K,
 $k = 0$, $\varepsilon = 0$

At the piston surface; $u_r = 0$, $u_y = U_{pis}(t)$, $T = T_{pis} = 360$ K,
 $k = 0$, $\varepsilon = 0$
 where D_H hydraulic radius, I turbulence density, l turbulence length scale.

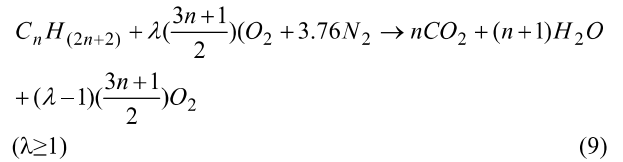
Spark plug energy was given 50 mJ in the spark timing

Combustion of fuel with air

Reaction mechanism: The simplest description of combustion is of a process that converts the *reactants* available at the beginning of combustion into *products* at the end of the process. In this study, the combustion of methane with oxygen is modeled with two-step reaction mechanism and the combustion of hydrogen with oxygen is modeled one step reaction mechanism. In the two-step reaction mechanism, the first stage, methane is oxidized into carbon monoxide and water vapor and in the second stage carbon monoxide oxidizes into carbon dioxide. The reaction mechanisms take place according to the constraints of chemistry, and are defined by:



The calculations are based on the mass fractions of components of mixtures and products according to the following combustion equation [17]:



COMPUTATIONAL PROCEDURE

Calculation tools

Even the difficult general differential equations are now yielding to the approximating technique known as numerical analysis, whereby the derivatives are simulated by algebraic relations between a finite numbers of grid points in the flow field which are then solved on a digital computer. The FLUENT 6.2 was chosen as the CFD computer code for this

work because of the ease with which the analysis model can be created, and because the software allows users to modify the code for special analysis conditions through the use of user subroutines. A variety of turbulence models is offered by the FLUENT computer code. The standart k-ε model was used as a turbulence model in this study. The model constants for the standart k-ε model are $C_{\mu}=0.09$, $C_{1\epsilon}=1.44$, $C_{2}=1.92$, $\sigma_k = 1.00$ and $\sigma_{\epsilon} = 1.30$.

Grid size: The grid independent tests were carried out to ensure grid independence of the calculated results; consequently, the grid size and the grid orientation giving the grid independent results were selected, and thus the total cell number of 85000 at the TDC and the total cell number of 200000 at the BDC was adopted.

NUMERICAL RESULTS

Validation of the Numerical Method

In order to achieve the validity of the numerical study, experimental study was realized with natural gas- hydrogen mixtures in Ford engine. Cylinder pressure values were compared with experimental results. Figure 2 shows comparison between the numerical cylinder pressures and experimental pressures at 2000 rpm and EAR 1.0. In this figures, numerical pressure values compare to experimental pressure values when the spark timing = 30° BTDC were investigated.

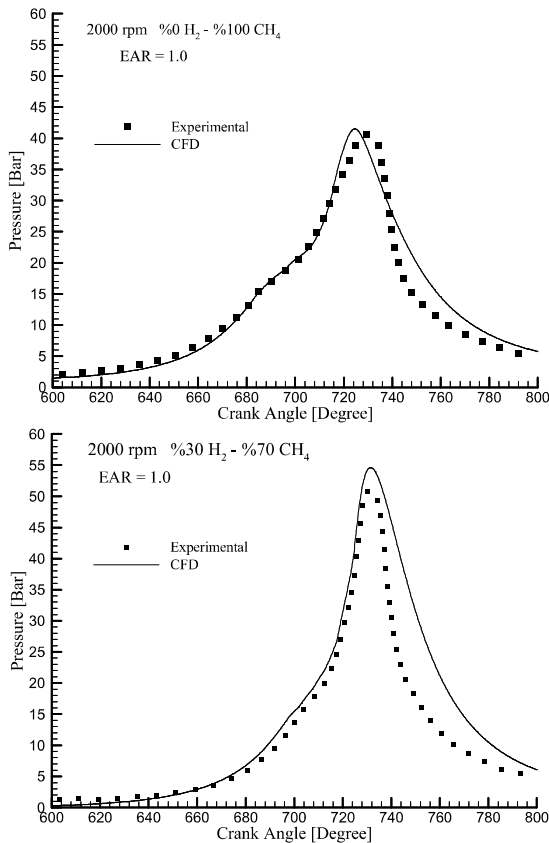


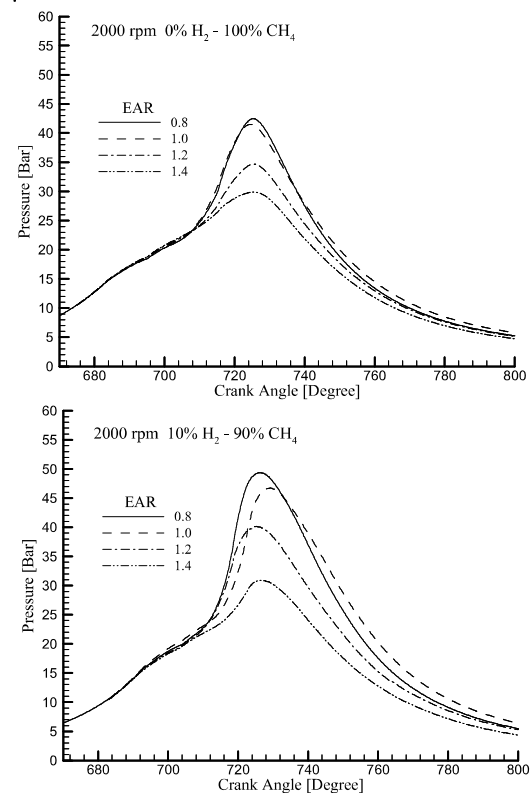
Figure 2 Cylinder pressures for %0H₂-%100 CH₄ and 30% H₂-70% CH₄ at 2000 rpm

The following parameters have been studied and varied as follows:

- Air excessive ratio (λ) has been varied from 0.8 to 1.4.
- Ignition advance is taken 30 CA BTDC
- H₂ addition to methane values are taken 0, 10, 20 and 30.
- Compression ratio (CR) has been considered 10.0.
- Spark plug energy has been taken 50 mJ.
- Engine speed has been taken 2000 rpm

Variation of Pressure in Cylinder

Figure 3 shows pressure values versus the crank angle with 30 spark timing, different H₂/CH₄ ratios and different excessive air ratios. As can be understood from these figures, the maximum pressure values are obtained at 30% H₂-70% CH₄ mixtures and excessive air ratio 0.8. In the case of excessive air ratio 1.0, 1.2 and 1.4, maximum pressure values are decreased. The maximum pressure values in the 30% H₂-70% CH₄ mixtures are obtained after top dead center (ATDC) 12. If combustion starts too early in the cycle, the work transfer from the piston to the gases in the cylinder at the end of the compression stroke is too large. If the combustion starts too late, the peak cylinder pressure is reduced, and the expansion stroke work transfer from the gas to the piston decreases. Thus, there exists a particular spark timing that gives maximum engine torque at fixed speed, mixture composition and flow rate. It is referred to as MBT or maximum brake torque timing.



2 Topics

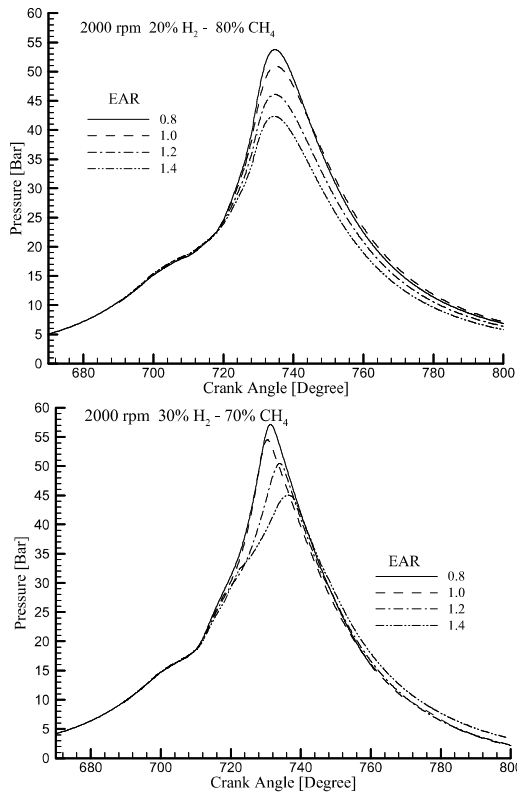


Figure 3 Cylinder pressures versus the crank angles for different natural gas-hydrogen mixtures and excessive air ratio at spark timing 30° BTDC.

Variation of Temperature in Cylinder

Figure 4 shows temperature values versus the crank angle with 30 spark timings different H₂/CH₄ ratios and different excessive air ratios. In this figures, temperature is increased after top dead center then decreased. Increasing the EAR, maximum temperature values are decreasing. The maximum temperature is obtained about 2400 K at 30% H₂-70% CH₄ and EAR=0.8. The minimum temperature values are observed in the EAR=1.4.

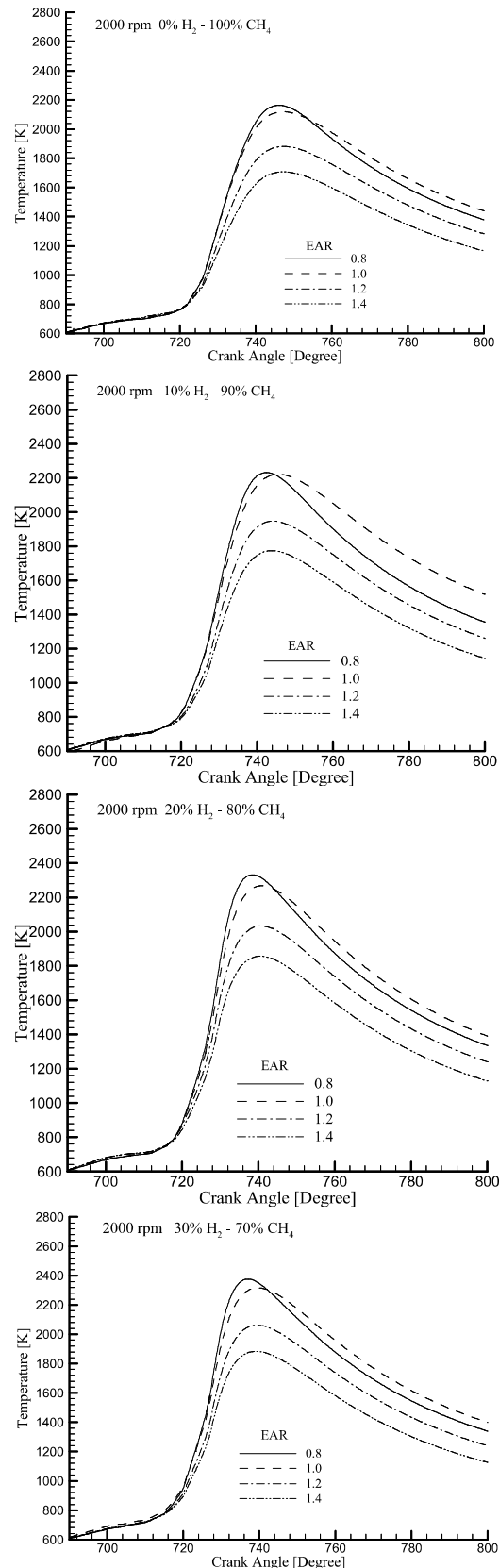


Figure 4 Temperature values versus the crank angles for different natural gas-hydrogen mixtures and excessive air ratio at spark timing 30° BTDC.

To achieve the highest levels of combustion efficiency, complete combustion should take place. Complete combustion occurs when all of the energy in the fuel being burned is extracted and none of the Carbon and Hydrogen compounds are left unburned. Complete combustion will occur when the proper amounts of fuel and air (fuel/air ratio) are mixed for the correct amount of time under the appropriate conditions of turbulence and temperature [18]. Figure 5 shows mass fractions of species for EAR=1 (CH₄, O₂, H₂O and CO₂) and 100% CH₄- 10% H₂- 90% CH₄ - 20% H₂- 80% CH₄ - 30% H₂- 70% CH₄. When the combustion initializes, CO₂ and H₂O values are rapidly increasing. The CO₂ and H₂O mass fractions of species after the spark plug are very rapidly increasing. Closing the spark timing TDC, O₂ mass fractions of species reaches higher values; CO₂, H₂O and CH₄ mass fractions of species are decreasing.

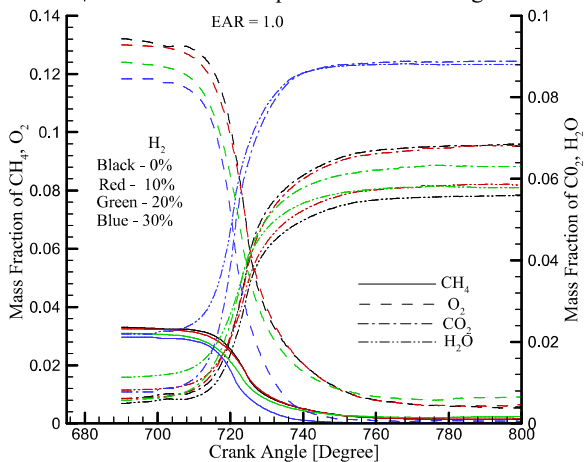


Figure 5 Mass fractions of species for EAR=1.0 (CH₄, O₂, H₂O and CO₂) (Spark timing=30)

Conclusions

The combustion of methane-hydrogen mixtures with air in a SI engine were considered to determine numerically the pressure, temperature and mass fraction of species in the combustion chamber. The effects of hydrogen addition to methane and excessive air ratio on the combustion also were investigated. The specific conclusions derived from this study can be listed briefly as follows:

- The increase of EAR reduces significantly the reaction rate levels.
- The maximum temperatures and maximum pressure values are obtained in %30 H₂-%70 CH₄ mixtures.
- The mass-weighted averages of the mass fractions of H₂O increase with decreases of EAR.
- The maximum temperature is obtained about 2400 K in 30 BTDC and 0.8 EAR.
- In case of EAR=1.0, the complete combustion occurs, and the combustion in the event of $\phi=1$ is very close to the complete combustion state.
- Maximum pressures are obtained EAR=0.8.

Consequently, the results of this study clearly demonstrate the numerical simulation of combustion of methane-hydrogen mixtures with air.

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