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Numerical Analyses of Combustion Methane-Hydrogen Mixtures in Cylinder for Different Spark Timing

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Preliminary note

In this study, numerical simulations of combustion characteristics using pure methane and 70 % CH₄-30 % H₂ blends were investigated in a spark ignition engine. The numerical calculations were performed using the finite volume CFD code FLUENT with standard *k-ε* model using the compression ratio and the engine speed are 10 and 2000 rpm respectively. Excess air ratios were selected as 1, 1.2 and 1.4. The spark timings were started at 45, 30 and 15 degree crank angle (CA) before top dead center (BTDC). The results of the combustion process were investigated as a function of crank angle. The maximum cylinder pressures and temperatures were obtained with 70 % CH₄-30 % H₂ mixture. It is observed that peak pressure values are decreased when the excess air ratio increased.

Numerička analiza izgaranja smjese metan –vodik u cilindru za različita vremena bacanja iskre

Prethodno priopćenje

U ovom se radu numerički simuliraju karakteristike izgaranja čistog metana i smjese 70 % CH₄ i 30 % H₂ kod motora paljenih sa svjećicom. Numerički proračuni su napravljeni koristeći kontrolni volumen CFD, kod FLUENT, sa standardnim *k-ε* modelom koristeći kompresijski omjer i brzinu motora 10 i 2000 min⁻¹. Odabrani faktori pretička zraka su 1, 1.2 i 1.4. Vrijeme početka paljenja iskom odgovaralo je 45, 30 i 15 stupnjeva koljenastog vratila prije gornje mrtve točke. Rezultati procesa izgaranja su istraživani u ovisnosti o kutu pretpaljenja. Utvrđeni su maksimalni tlakovi u cilindru za smjesu 70 % CH₄ i 30 % H₂. Uočeno je da se smanjuju vrijednosti maksimalnog tlaka s povećanjem faktora pretička zraka.

1. Introduction

Today, energy which is needed for the function of a motor vehicle can execution largely dependent petrol. Therefore, problems at fuel getting are increasing with the fixed rapid increases of fuel consumption. Also, air pollution and noise level resulting from motor vehicles, especially in big cities, is a crucial problem and has already reached human health threatening size. Pollution of the air eliminated or diminished minimum level, it is possible that decreasing fuel consumption and increase efficiency of motor vehicle <http://www.modifyliarabalar.net>.

[1] has introduced the preliminary simulation of a four stroke spark ignition engine. An arbitrary heat release formula is used to predict the cylinder pressure, which is used to find the indicated work done. The heat transfer from the cylinder, friction and pumping losses also are 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 that seen for the real engine. The modeling process is obviously getting closer to reality and is now worth pursuing as a design aid.

[2, 6, 11] researched on utilization of natural gas-hydrogen mixtures in internal combustion engine. They concluded that hydrogen is the best gaseous candidate for blending with natural gas. They found that natural gas-hydrogen mixtures have decreased exhaust emission and efficiency might have been increased under certain conditions.

[8] a mathematical simulation model is developed to investigate ideal air-fuel cycle analysis of a single cylinder, four-stroke and natural aspirated spark ignition engine. Variations of cylinder temperature and pressure with crankshaft angle (CA) depending on different compression ratio were obtained along with, engine speed and air excess coefficient (AEC); engine performance parameters such as indicated mean effective pressure, fuel and air consumptions, indicated power, thermal efficiency are calculated using a computer program written in FORTRAN. Iso- Octane (C₈H₁₈) is

Symbols/Oznake			
ST	- Spark Timing početak paljenja	C_ξ	- volume fraction constant - konstanta volumenskog udjela
BTC	- Bottom dead center - donja mrtva točka	ν	- kinematic viscosity - kinematička viskonost
CFD	- Computational Fluid Dynamics - računalna dinamika fluida	C_T	- time scale constant - konstanta vremenskog ramjera
CA	- Crank Angle - kut zakreta radilice	Y_i^+	- fine-scale species mass fraction - fini – razmjer masenog udjela sudionika
EAR	- Excess air ratio - faktor pretička zraka	D_H	- hydraulic radius - hidraulički radijus
TDC	- Top Dead Center - gornja mrtva točka	I	- turbulence density - turbulentna gustoća
BTDC	- before top dead center - prije gornje mrtve točke	l	- turbulence length scale - razmjer turbulentne duljine
ATDC	- after top dead center - poslije gornje mrtve točke		

used as a fuel in the numerical calculation method, and calculation of internal energy and specific heats belong to C_8H_{18} and species and calculation of considered two basic dissociation equilibrium constants are determined as the empiric functions of temperature. It is assumed that combustion and exhaust processes are done at constant volume and compression, combustion and expansion processes are adiabatic. With these results, it is believed that the mathematical model can be used for determination of engine performance characteristics as an appropriate method in internal combustion engines.

[10] has been simulated a hydrogen internal combustion engine Ricardo WAVE used in Texas Tech Universities Future Truck Ford Explorer in the master's thesis. Initially, a naturally aspirated gasoline engine is simulated, followed by the supercharged hydrogen engine. The objective of these simulations is to maximize power of the hydrogen engine, while minimizing the emissions and fuel consumption. Among the variables which are changed, are the equivalence ratio, compression ratio, throttle opening, camshaft timing, and exhaust size. The simulation results studied included the volumetric efficiency, fuel consumption, as well as NO emissions. The highest fuel efficiency is given by approximately 14.5:1 to 15:1 compression ratio for a naturally aspirated model, and approximately 12.5:1 to 13:1 for the supercharged model.

[12] has been described to accurately predict the gas pressure changes within the cylinder of a spark-ignition engine using thermodynamic principles. The model takes into account the intake, compression, combustion, expansion and exhaust processes that occur in the cylinder. Comparisons with actual pressure data show

the model to have a high degree of accuracy. The model is further evaluated on its ability to predict the angle of spark firing and burn duration.

Shidfar and Garshasbi 2005, have presented a differential model of in-cylinder pressure in an internal combustion engine. For this purpose, the compression stroke analyzed and Fourier law was used to model the cylinder pressure. An unknown function appears in the coefficient of this equation. This unknown function is approximated by cubic B-spline. To estimate unknown parameters, the modified Levenberg–Marquardt algorithm is used. The numerical solution of the direct problem is used to simulate pressure measurement.

Traditionally, to improve the lean-burn capability and flame burning velocity of the natural gas engine under lean-burn conditions, an increase in flow intensity in cylinder is introduced, and this measure always increases the heat loss to the cylinder wall and increases the combustion temperature as well as the NO_x emission [7]. One effective method to solve the problem of slow burning velocity of natural gas is to mix the natural gas with the fuel that possesses fast burning velocity. Hydrogen is regarded as the best gaseous candidate for natural gas due to its very fast burning velocity, and this combination is expected to improve the lean-burn characteristics and decrease engine emissions [2].

In the present work, a two-dimensional model was developed to simulate a 4-stroke cycle of a spark ignition engine fueled with methane and methane hydrogen mixture depending on crankshaft angle. In order to investigate the effect of spark timing and excess air ratios on the combustion, the combustion phenomena is examined by using Fluent CFD code [9].

2. Mathematical Model

2.1. Cylinder Geometry

In this study, a variation of temperature and pressure for different spark timings and different excess air ratios in cylinder has been estimated. For this purpose, the combustion of methane (100 % CH₄) and methane-hydrogen (70 % CH₄-30 % H₂) mixtures in a cylinder have been considered. Spark timing ratio has been selected from 45, 30 and 15 CA BTDC and excess air ratio (λ) has been taken 1, 1.2, and 1.4. The two-dimensional model and dimensions of this considered cylinder are shown in Figure 1. Crank shaft speed is taken 2000 rpm. The main geometrical details of the engine are as given in Table 1. As apparent from this figure, the methane- hydrogen mixtures enters the intake valve and the burned gas exits the exhaust valve. The piston moves from TDC to BDC.

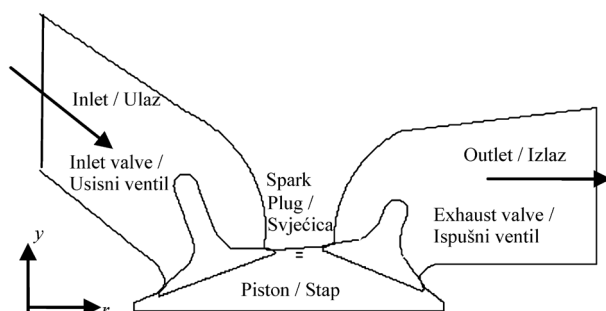


Figure 1. Two dimensional cylinder geometry

Slika 1. Dvodimenzionalna geometrija cilindra

Table 1. Engine specifications

Tablica 1. Specifikacije motora

Bore / Unutrašnji promjer	80.6	mm
Stroke / Hod	88	mm
Compression Ratio / Kompresijski omjer	10:1	-
Exhaust valve opening / Otvaranje ispušnog ventila	55°	BBDC
Exhaust valve closing / Zatvaranje ispušnog ventila	50°	ATDC
Intake valve opening / Otvaranje usisnog ventila	13°	BTDC
Intake valve closing / Zatvaranje usisnog ventila	47°	ABDC
Intake valve radius / Polumjer usisnog ventila	30°	mm
Exhaust valve radius / Polumjer ispušnog ventila	28°	mm

The spark plug is settled in the middle of intake and exhaust manifold. Spark plug energy is given 50 J in the

spark timing. While cycle come true, intake and exhaust valve are opened and closed by depending on the crank angle. At the compression stroke, while the piston closed the TDC spark energy is given at the different point (BTDC 45°, 30° and 15° CA). At this time intake and exhaust valve is closed condition. FLUENT 6.2 program is used as CFD computer code [9].

2.2. Mathematical model

The models and assumptions used for the numerical calculations are as follows:

- For the turbulent flow, the “standard $k-\epsilon$ model”
- For the chemical species transport and reacting flow, the eddy dissipation concept with the diffusion energy source option.
- The flow is steady, two-dimensional and compressible.
- The fuel-air mixture is assumed as ideal gas.
- Cylinder walls are constant temperature.
- PRESTO algorithm is used as solution technique
- PISO is taken pressure-velocity coupling scheme

2.2.1. 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:

$$\zeta^* = C_\xi \left(\frac{\nu \epsilon}{k^2} \right)^{3/4}, \quad (1)$$

where * 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

$$\tau^* = C_\tau \left(\frac{\nu}{\epsilon} \right)^{1/2}, \quad (2)$$

where C_τ is a time scale constant equal to 0.4082.

The source term in the conservation equation for the mean species i ,

$$R_i = \frac{\rho (\zeta^*)^2}{\tau^* [1 - (\zeta^*)^3]} (Y_i^* - Y_i), \quad (3)$$

where Y_i^* is the fine-scale species mass fraction after reacting over the time τ^* .

2.2.2. Physical properties and engine values

Intake valve radius $r_{\text{intake}} = 16$ mm, exhaust valve radius $r_{\text{exhaust}} = 14$ mm, cylinder diameter $D = 80.6$ mm,

piston stroke $H=88$ mm, connecting rod length $l=132$ mm, $T_{ref}=300$ K, Methane and Methane- hydrogen mixtures are assumed ideal gas and taken properties from FLUENT Material Properties Database [9].

Boundary conditions:

At the intake valve; $u_x=U_y$ and $T=T_{in}=300$ K,
 $l=0.07 D_H$,

$$k = \frac{3}{2} (IU_{int})^2 \text{ and } \varepsilon = C_\mu^{3/4} \frac{k^{3/2}}{l}. \quad (4)$$

At the exhaust valve; Pressure outlet=atmospheric medium

At the cylinder wall;

$$u_r=0, u_y=0, \quad T=T_d = 360 \text{ K}, \quad k=0, \quad \varepsilon=0$$

At the piston surface;

$$u_r=0, u_y=U_{pis}(t), \quad T=T_{pis}=360 \text{ K}, \quad k=0, \quad \varepsilon=0,$$

where D_H hydraulic radius, I turbulence density, l turbulence length scale.

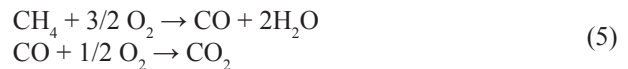
Spark plug energy was given 50 J in the spark timing.

2.3. Combustion of fuel with air

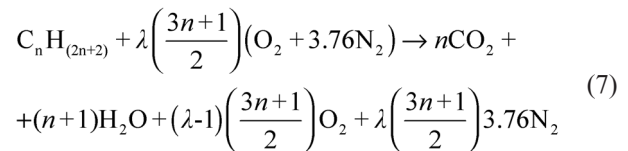
2.3.1. Reaction mechanism

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 [4]:



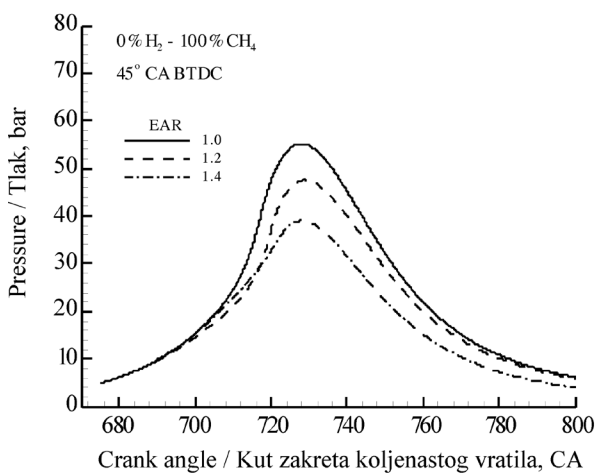
Where λ is excess air ratio. Excess air ratio which describes the mixture ratio, burning speed is affected because of the heat amount which emerges, variation of pressure and temperature.

2.3.2. Grid size

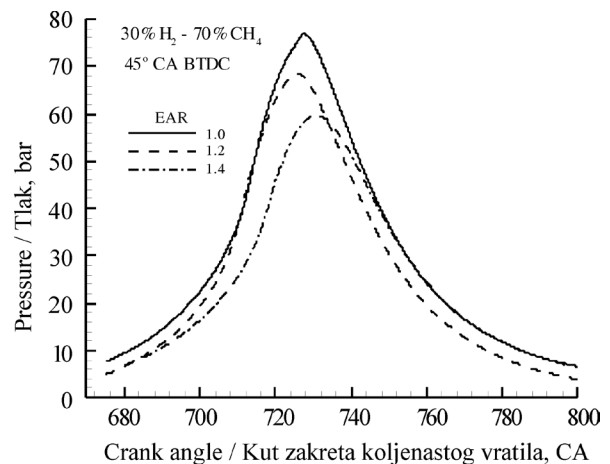
The grid independent tests were carried out to ensure grid independence of the calculated results; consequently, the grid size and the grid orientation giving the grid independent results were selected, and thus the total cell number of 85000 at the TDC and the total cell number of 220000 at the BDC was adopted.

3. Numerical Results

Figure 2 and Figure 4 shows variations of pressure in the cylinder at 45, 30 and 15 degree CA spark timing, EAR 1.0, 1.2 and 1.4 values for 100 % CH_4 and 70 % CH_4 - 30 % H_2 mixtures. The highest pressure value is obtained at BTDC 45 degree CA and 70 % CH_4 - 30% H_2 mixtures at EAR 1.0. Maximum pressure values are



a)



b)

Figure 2. Variations of pressure values versus crank angle at 45 degree CA

Slika 2. Vrijednosti tlaka u ovisnosti o kutu radilice za kut paljenja 45°.

decreased with increased EAR. In the case of hydrogen adding to methane, because hydrogen has high heat value, highest maximum pressure values are obtained at 70 % CH₄ - 30 % H₂ mixtures. It is shown that maximum pressure values are decreased with the spark timing closed at TDC. Maximum pressure values are generally desired at about 7 MPa in spark ignition engine [13]. This value is obtained approximately 56 bar at 45 degree CA, EAR 1.0 for 100 % CH₄ and 80.15 bar for 70 % CH₄ - 30 % H₂ mixtures respectively.

Figure 5, 6 and 7 show temperature values versus the crank angle with 1, 1.2 and 1.4 excess air ratios at 45, 30 and 15 degree CA spark timing, respectively. Closing the spark timing TDC and increasing the EAR, maximum temperature values are decreasing. For 100 % CH₄ maximum temperatures are obtained approximately

2271 K at EAR 1.0 and spark timing 45 degree CA. For 70 % CH₄ - 30 % H₂ maximum temperatures are obtained approximately 2806 K at EAR 1.0 and spark timing 45 degree CA. In case of EAR 1.0 and spark timing 30 degree CA maximum temperature values are obtained 1998 K and 2339 K for 100 % CH₄ and 70 % CH₄ - 30 % H₂ mixtures respectively. In these conditions temperature values are increasing with the adding of hydrogen to methane. Because hydrogen has higher heat values than methane. Table 2 and Table 3 are shown variation of pressure and temperature values at maximum point. From Table 2 and Table 3, pressure and temperature values are decreased with the spark timing close the TDC and increase the EAR. 100 % CH₄ values are lower than 70 % CH₄ - 30 % H₂ mixture values.

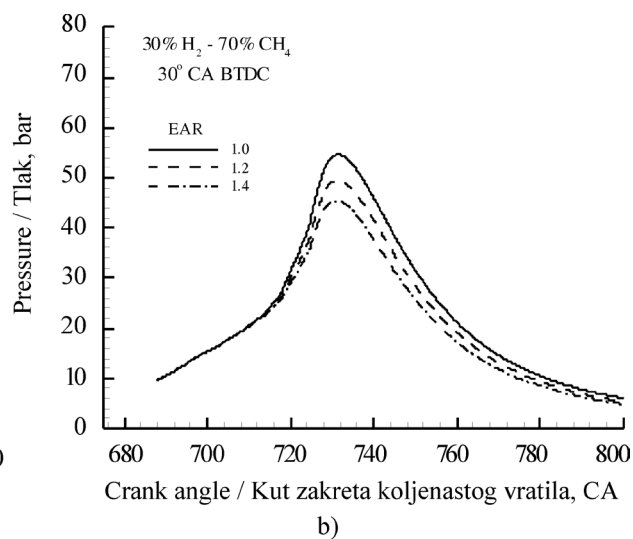
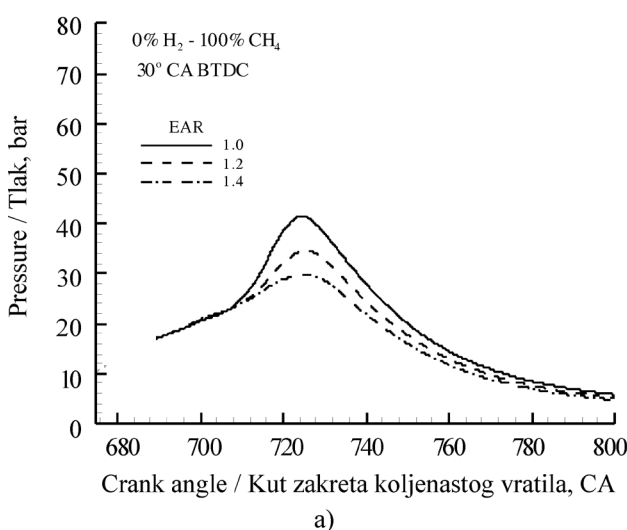


Figure 3. Variations of pressure values versus crank angle at 30 degree CA

Slika 2. Vrijednosti tlaka u ovisnosti o kutu radilice za kut paljenja 30°.

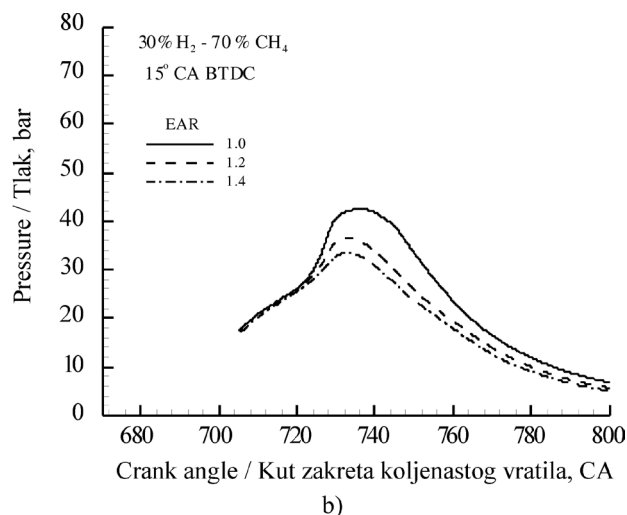
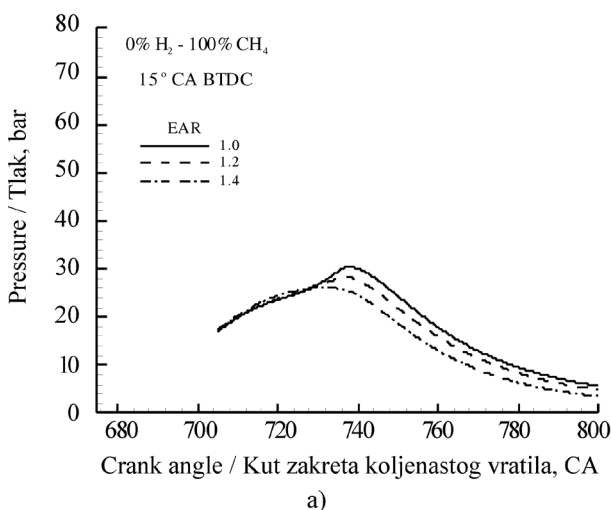


Figure 4. Variations of pressure values versus crank angle at 15 degree CA

Slika 4. Vrijednosti tlaka u ovisnosti o kutu radilice za kut paljenja 15°.

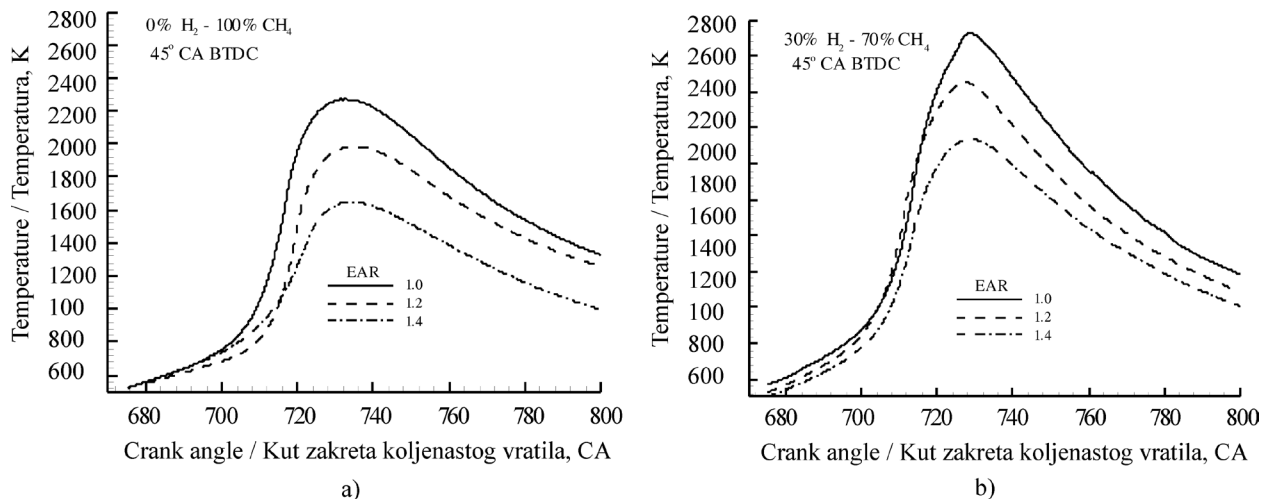


Figure 5. Variation of temperature values versus CA at 45 degree CA

Slika 5. Vrijednosti temperature u ovisnosti o kutu radilice za kut paljenja 45°

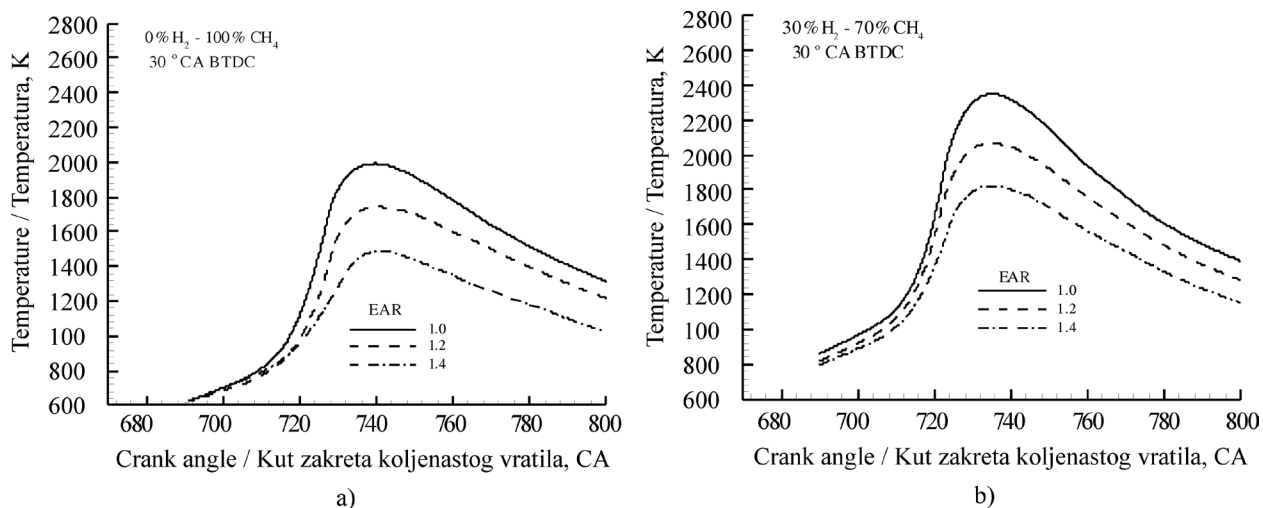


Figure 6. Variation of temperature values versus CA at 30 degree CA

Slika 6. Vrijednosti tlaka u ovisnosti o kutu radilice za kut paljenja 30°

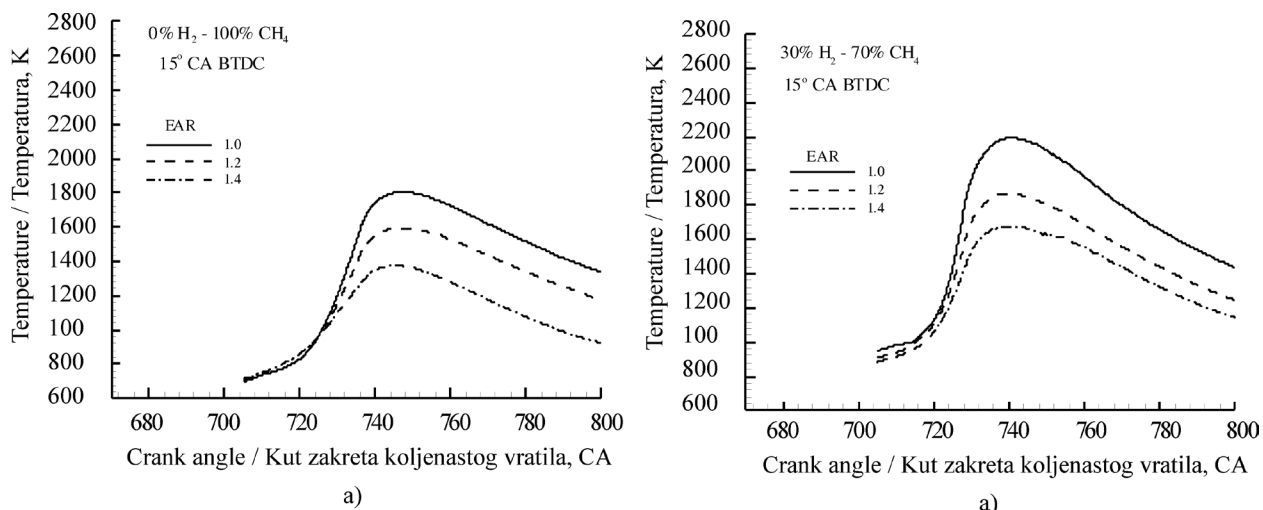


Figure 7. Variation of temperature values versus CA at 15 degree CA

Slika 7. Vrijednosti temperature u ovisnosti o kutu radilice za kut paljenja 15°.

Table 2. Maximum pressure and temperature values for 100 % CH₄

Tablica 2. Vrijednostim maksimalnih tlakova temperature a 100 % CH₄

Spark timing	EAR=1.0		EAR=1.2		EAR=1.4	
	Pressure / Tlak, MPa	Temperature / Temperatura, K	Pressure / Tlak, MPa	Temperature / Temperatura, K	Pressure / Tlak, Mpa	Temperature / Temperatura, K
45 ° CA	54.9	2271	47.6	1977	39.1	1652
30 ° CA	41.2	1998	34.4	1736	30.0	1479
15 ° CA	29.8	1804	28.2	1593	25.8	1372

Table 3. Maximum pressure and temperature values for 70 % CH₄ - 30 % H₂

Tablica 3. Vrijednosti maksimalnih tlakova temperature za 70 % CH₄ - 30 % H₂

Spark timing	EAR=1.0		EAR=1.2		EAR=1.4	
	Pressure / Tlak, Mpa	Temperature / Temperatura, K	Pressure / Tlak, Mpa	Temperature / Temperatura, K	Pressure / Tlak, Mpa	Temperature / Temperatura, K
45 ° CA	77	2725	68.1	2449	59.8	2132
30 ° CA	54.4	2339	49.12	2061	45.28	1814
15 ° CA	42.9	2232	36.4	1870	33.3	1674

Figure 8, 9 and Figure 10 show variation of mass fraction of reactant and product of reaction for 100 % CH₄ and 70% CH₄ - 30 % H₂ mixtures at EAR 1.0 and spark timing 45, 30 and 15 degree CA. With the beginning of burning mass fraction of CH₄ and O₂ values are decreased and mass fraction of CO₂ and H₂O product values are increased.

4. Conclusions

The specific conclusions derived from this study can be listed briefly as follows:

- Engine performances are affected with the spark timing.
- With the increase of EAR, low pressure and low temperature values are obtained at the lean mixtures.

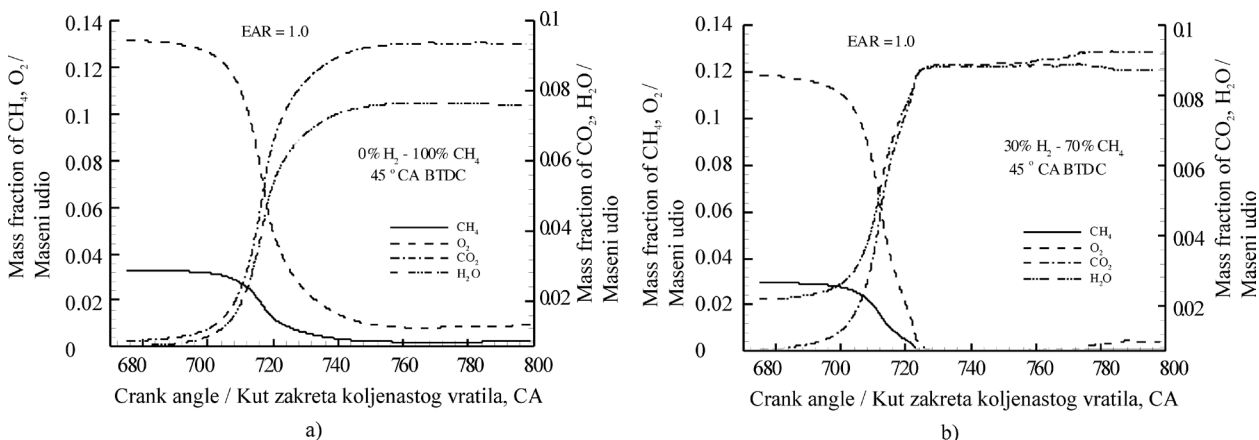


Figure 8. Mass fraction of species versus crank angle at BTDC 45 degree CA

Slika 8. Maseni udio sudionika u ovisnosti o kutu radilice pri kutu paljenja 45°

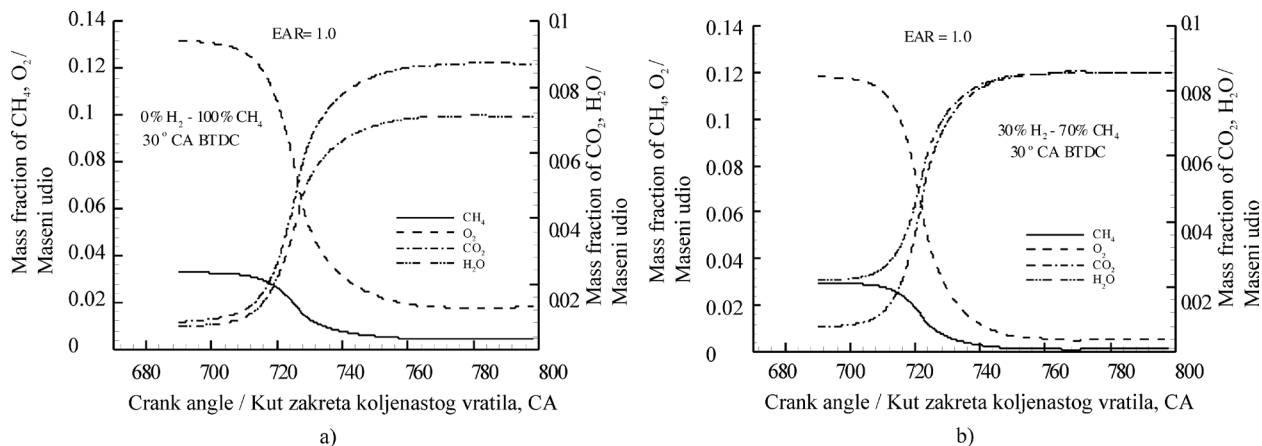


Figure 9. Mass fraction of species versus crank angle at BTDC 30 degree CA

Slika 9. Maseni udio sudionika u ovisnosti o kutu radilice pri kutu paljenja 30°

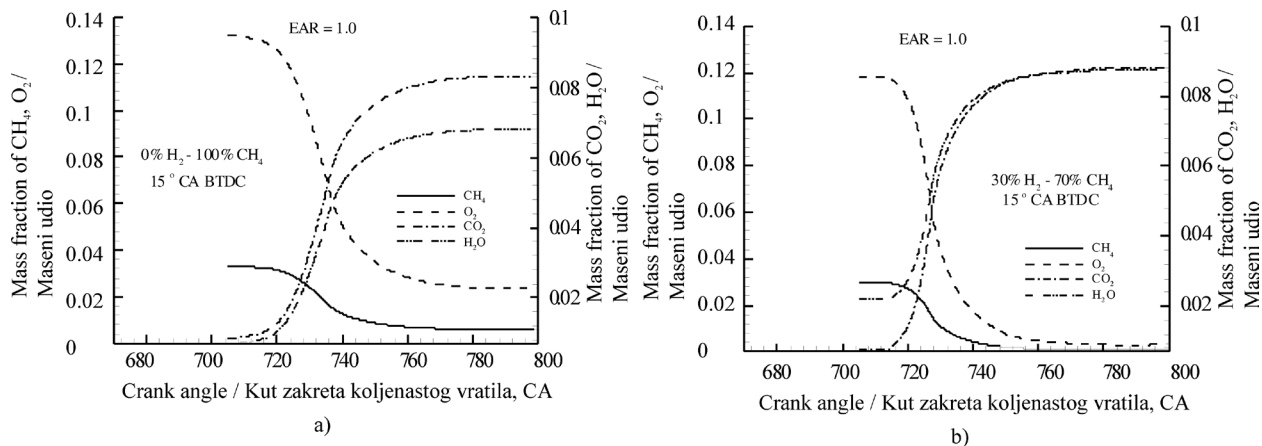


Figure 10. Mass fraction of species versus crank angle at BTDC 15 degree CA

Slika 10. Maseni udio sudionika u ovisnosti o kutu radilice pri kutu paljenja 15°

- In case of adding hydrogen to methane, high pressure and temperature values are obtained.
- With the reduction of temperature and pressure values result reduction of mass fraction of species and products.

Consequently at future studies, optimization can be performed with the parameters applied in this study by varying engine speed, compression ratio, spark timing for lean mixtures and EAR for rich mixtures.

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