

Effects of mass flow rate and equivalence ratio on laminar premixed methane air flame

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Geliş / Received: 04/08/2020, Kabul / Accepted: 01/03/2021

Abstract

The structures of laminar premixed flames of methane air mixture are investigated for different equivalence ratios and different mass fluxes numerically. Equivalence ratio values are taken as 0.6, 1 and 1.4 that can be seen in engineering applications. These values correspond to lean, stoichiometric and rich methane-air mixtures respectively. CHEMKIN 19 program and GRI-Mech 3.0 mechanism are used for numerical solution. The axial velocity and mole fractions of CH₄ and O₂ as reactants, and mole fractions of H₂O, CO, CO₂ and H₂ as products are investigated for each runs. It is found that with the increase of the mass flow rate; the axial velocities of the flame, the axial location of the reaction zones and the mole fraction values of the intermediates increases. The values of the mole fractions of the reactants do not change with mass flux.

Keywords: Methane-air mixture, laminar premixed flame, equivalence ratio

Kütle debisi ve denklik oranlarının ön karışımli laminar metan-hava karışımı alevi üzerine etkileri

Öz

Metan hava karışımından oluşan laminer ön karışımli alev yapısı farklı denklik oranı ve farklı kütle debileri için sayısal olarak incelenmiştir. Mühendislik uygulamalarında görülen değerler olarak denklik oranları 0,6, 1 ve 1,4 olarak seçilmiştir. Bu değerler sırasıyla fakir, stokiyometrik ve zengin metan hava karışımı değerlerine karşılık gelmektedir. Kütle debileri olarak 0,01, 0,1 ve 0,3 g/cm²s seçilmiştir. Sayısal çözümleme için CHEMKIN 19 programı ve GRI-Mech 3.0 mekanizması kullanılmıştır. Her bir deneme sonucunda alevin eksenel hızı ve reaksiyona giren CH₄ ile O₂ ve reaksiyon sonucunda H₂O, CO, CO₂ ve H₂ nin mol oranları belirlenmiştir. Sonuç olarak, kütle debisi arttıkça, alevin eksenel hızının arttığı, reaksiyon bölgesinin eksenel konumunun ve ara bileşiklerin mol oranlarının arttığı belirlenmiştir. Ayrıca kütle debisinin değişmesi ile ürünlerin mol oranlarının değişmediği görülmüştür.

Anahtar Kelimeler: Metan-hava karışımı, laminar ön karışımli alev, denklik oranı

1. Introduction

Combustion is the process of the exothermic reactions between a fuel and oxidant. It can be said that the most important classification of combustion is the flame type. Flames can

be separated into two types. One of them is premixed and the other is non-premixed. A

Bunsen burner is a very good example where both type of flames are produced. Air and

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fuel are mixed in the mixing tube. This premixed mixture burns, forming a conical flame of finite thickness. This is called premixed flame (Date, 2011).

Methane is a primary reference fuel. It was studied in the previous works for understanding the fundamental combustion characteristics in terms of ignition delay, flame propagation speed, flame instabilities and dynamic behaviors (Varghese et al. 2017).

There are many previous works concerning about the structure of laminar premixed flames. Detailed literature survey can be found in the thesis of Wu(2016), Maleta (2017) and Hu (2013). Especially the thesis of Maleta (2017) gives detailed knowledge on the subject of burner stabilized laminar flame and the paper of Cardona et al.(2013) is a good source for literature review.

An early paper was presented by Botha and Spalding (1954) for measurement of flame speed of propane air mixture experimentally. The flame was stabilized over a wide range of mixture ratio and with flame speeds ranging between 4 and 38 cm/s. The experimental results were also compared with literature.

Ren et al. (2020) investigated the one dimensional premixed freely propagating flames of $\text{CH}_4+(\text{CO}_2/\text{H}_2\text{O})$ / air mixtures by using Chemkin II/premixed code. The effects of addition of CO_2 and steam on the mixture were found. The formations of intermediates were determined and a detailed analysis was given.

The soot formation and evolution characteristics in premixed methane/ethylene oxygen, argon flames were studied experimentally and numerically by Liu et

al.(2019). Smooke (1982), developed a numerical technique for integrating the one-dimensional steady state premixed laminar flame equations. A global finite difference approach was used in which the nonlinear difference equations were solved by a damped-modified Newton method. Mendes et al. (2008) studied a 1D model to simulate combustion within porous media and a linear stability analysis was performed. A linearized version of the discrete-ordinates radiation model was included in the linear stability analysis to discuss the stability of submerged and surface steady flames. In addition, the influence of the various treatments of the solid/gas interface at inlet and outlet porous planes and radiation models on the stability of the calculated flames were discussed. Hu et al. (2017) worked on laminar methane-air premixed Bunsen flame by using numerical simulations and laser diagnostics. They showed that the inlet velocity of the burner affects the accuracy of the generated laminar flame speed as a conclusion. It was suggested that a suitable inlet velocity of methane-air mixture was approximately six times the laminar flame speed. The structures of three laminar premixed stoichiometric flames at low pressure a pure methane flame, a pure ethanol flame and a methane flame doped by 30% of ethanol, have been investigated and compared by Tran et al. (2013). The laminar flame velocity of natural gas, methane, ethane, propane and n-butane and also binary and tertiary mixtures of these compounds is determined by Dirrenberger et al. (2011) experimentally. The experiments were performed at atmospheric pressure in an adiabatic burner. The equivalence ratios were taken in a wide range from 0.6 to 2.1, due to satisfy a stabilized flame. The experimental data were compared with empirical correlations and chemical mechanisms. A

paper concerning about turbulent premixed methane flame diluted by carbon dioxide at atmospheric and elevated pressures can be published by Slefarski (2019). The influences of fluid properties and operation parameters on the emission of NO_x , CO and flame properties were investigated numerically and experimentally. The range of equivalence ratio was taken as 0.42 to 0.85. It is reported that NO_2 was doubled when the pressure were increased. CO emission raised with the CO_2 content in the fuel.

In this paper the axial velocity and mole fractions of fuel, oxidizer and intermediates are obtained by using CHEMKIN 19 Program (Chemkin-Pro,2011) and GRI-Mech 3.0 mechanism for burner stabilized methane air mixture numerically. Three different equivalence ratios are taken as 0.6, 1 and 1.4. The value 0.6 corresponds to lean, stoichiometric and rich methane-air mixtures respectively. The length of the solution domain is taken as 10 cm and the pressure is assumed as 1 atm. Three different mass fluxes are considered (0.01, 0.1 and 0.3 $\text{g}/\text{cm}^2\text{s}$). The fuel, oxidizer and intermediate species mole fractions are determined.

2. Material and Methods

In combustion, the air is generally used as the oxidant and, on a molecular level, it is thought to consist of 79% nitrogen and 21% oxygen. The Bunsen burner, patented in 1855, is possibly the most popular device for generating laminar premixed flames in a laboratory. (Kuo,2005). In this burner, near the bottom, fuel gas enters via a feed line. In the mixing tube, air and fuel are combined. This premixed fuel and air combination burns to create a conical flame. Near the peak of the burner, the flame is grounded. The premixed flame can stay stagnant as long as the fuel feeding rate stays steady. The fuel-

air mixture moves low enough at a velocity to ensure laminar flow conditions (Date, 2011).

There is a luminous conical region in the premixed laminar flame where reaction and heat release occurs. The luminous zone is roughly 1 mm thick. The color of the luminous region varies with the air/fuel combination. When the mixture is fuel-rich, the cone's color turns to green, and when the mixture is fuel-lean, the cone's color is dark violet. (Kuo,2005)

Mathematically, the equivalence ratio is described as;

$$\phi = \frac{F/O}{(F/O)_{st}} \quad (1)$$

In this equation, ϕ is the equivalence ratio, F/O reflects the ratio of fuel to oxidant, and the subscript st signifies the stoichiometric conditions. The mixture of fuel-oxidant is considered lean when the equivalence ratio is less than one, indicating "too much" oxygen. In the equivalence ratio being greater than one, the fuel-oxidant mixture is said to be rich; thus, there is excess fuel.

A premixed flame structure has two distinct zones: the pre-heat zone and the reaction zone. The reaction takes place steadily in the pre-heat zone and produces just a limited amount of heat. Nevertheless, fuel and oxidizer react rapidly in the reaction region, which releases the bulk of the heat and generates intermediate species. Consequently, the fast reaction zone is comparatively small, normally less than a millimeter at atmospheric pressure. The concentration and temperature gradients of organisms are very wide in this thin region, and heat diffusion flows back to the pre-heat zone due to these gradients' activation

energy, allowing the flame to self-sustain. (Hu, 2013).

Typically, the chemical combustion process is modeled by the burner-stabilized laminar premixed flames studied. Many combustors depend on the propagation of the premixed flame.

The conservation equations can be written for one-dimensional flow with standardized inlet conditions as follows: (Chemkin-Pro, 2011);

The continuity equation,

$$\dot{m} = \rho u A \quad (2)$$

Here; \dot{m} is the mass flow rate, ρ is the density, u is the fluid mixture velocity, A is cross-sectional area of the stream tube.

The energy equation,

$$\begin{aligned} \dot{m} \frac{dT}{dx} - \frac{1}{c_p} \frac{d}{dx} \left(\lambda A \frac{dT}{dx} \right) + \\ \frac{A}{c_p} \sum_{k=1}^K \rho Y_k V_k c_{pk} \frac{dT}{dx} + \frac{A}{c_p} \sum_{k=1}^K \dot{\omega}_k h_k W_k + \\ \frac{A}{c_p} \dot{Q}_{rad} = 0 \end{aligned} \quad (3)$$

Here, T is temperature, x is coordinate, c_p is the mixture's specific heat at constant pressure, λ is thermal conductivity, Y_k is mass fraction, V_k , k th species diffusion velocity, $\dot{\omega}_k$, molar rate of output by k th species chemical reaction per unit length, h_k , k th species basic enthalpy, W_k , k th species molecular weight, \dot{Q}_{rad} , thermal radiation heat loss.

The conservation of species,

$$\dot{m} \frac{dY_k}{dx} + \frac{d}{dx} (\rho A Y_k V_k) - A \dot{\omega}_k W_k = 0 \quad (4)$$

And the equation of state,

$$\rho = \frac{P \bar{W}}{RT} \quad (5)$$

Here, \bar{W} is the mixture's molecular weight, R universal gas constant, P pressure.

The reaction proceeds are assumed in the Arrhenius form,

$$k_f = AT^\beta \exp\left(\frac{E_A}{RT}\right) \quad (6)$$

Here; k_f is forward rate coefficient, β is temperature exponent, E_A is the activation energy.

The mixture's diffusion velocity V_k is composed of three parts,

$$V_k = v_k + W_k + V_c \quad (7)$$

v_k is the ordinary diffusion velocity, V_c is the velocity of correction, (Curtiss-Hirschfelder, 1954). v_k can be found as,

$$v_k = -D_{km} \frac{1}{X_k} \frac{dX_k}{dx} \quad (8)$$

and the average diffusion coefficient D_{km} of the mixture is given as,

$$D_{km} = \frac{1-Y_k}{\sum_{j \neq k}^K \frac{X_j}{D_{kj}}} \quad (9)$$

Here, X_k is the mole fraction and D_{kj} is the coefficient of binary diffusion.

The conservation equations govern the the two different forms of flames: burner stabilized flames and adiabatic freely propagating flames. For these forms, however, the boundary conditions are different.

\dot{m} is known priory and constant for burner stabilized flames. The temperature and mass flux fractions are specified at the cold boundary, and vanishing gradients are imposed at the hot boundary (Kee, 1998).

The methane air mixtures are calculated for the following conditions.

- Equivalence ratios are 0.6,1 and 1.4.
- Pressure is 1 atm
- Mass fluxes of the fuel is 0.01, 0.1 and 0.3 g/cm²s
- The domain is 10 cm
- The maximum number of grid points taken is 250
- Absolute tolerance is 1.0E-10
- Relative tolerance is 0.0001

3. Results and Discussions

Figure 1 shows the axial velocity of the flame for various mass flow rates of the stoichiometric methane air mixture. It can be seen that with the increase of the mass flow rate the axial velocity increases. The characteristics of the curves are similar to each other. The velocity curves make a leap at the reaction zone. As can be seen from Fig. 1.a the leap at the curve of $\dot{m}=0.01$ g/cm²s is at a distance of 1 -2 cm from the inlet. For $\dot{m}=0.1$ g/cm²s, the reaction zone occurs at a distance of 4-5 cm from the inlet. Finally for $\dot{m}=0.3$ g/cm²s it is between 5-7.5cm. If Fig. 1.a and Fig. 1.b are compared with each other, as the mass flow rate increases 10 times, the axial velocity also increases 10 times proportionally at the similar axial locations. It can be seen from Fig.1.b and Fig 1.c, when the mass flow rate is tripled, the axial velocities triples also. The mole fraction of the reactants, products and intermediates are shown for $\dot{m}=0.01$ g/cm²s at Figure 2. While the abscissa shows the axial distance, the ordinate shows the mole fractions. Fig. 2a is given for the lean mixture of methane and air ($\phi=0.6$). Fig. 2.b is drawn for stoichiometric mixture ($\phi=1$), and Fig.2.c is

for rich mixture ($\phi=1.4$). It can be seen from Fig.2 that the reaction occurs at an axial distance of 1 to 2 cm. As can be seen from Fig. 2.b the reactants CH₄ and O₂ completely transformed into the products H₂O, and CO₂. It can be seen from Fig. 2.a that whether the methane air mixture is assumed as lean or not, there is always O₂ at oxidation layer as expected. From Fig. 2.c it can be observed that the rich mixture reactants CH₄ and O₂ completely transformed into the products of H₂O, CO, CO₂ and H₂.

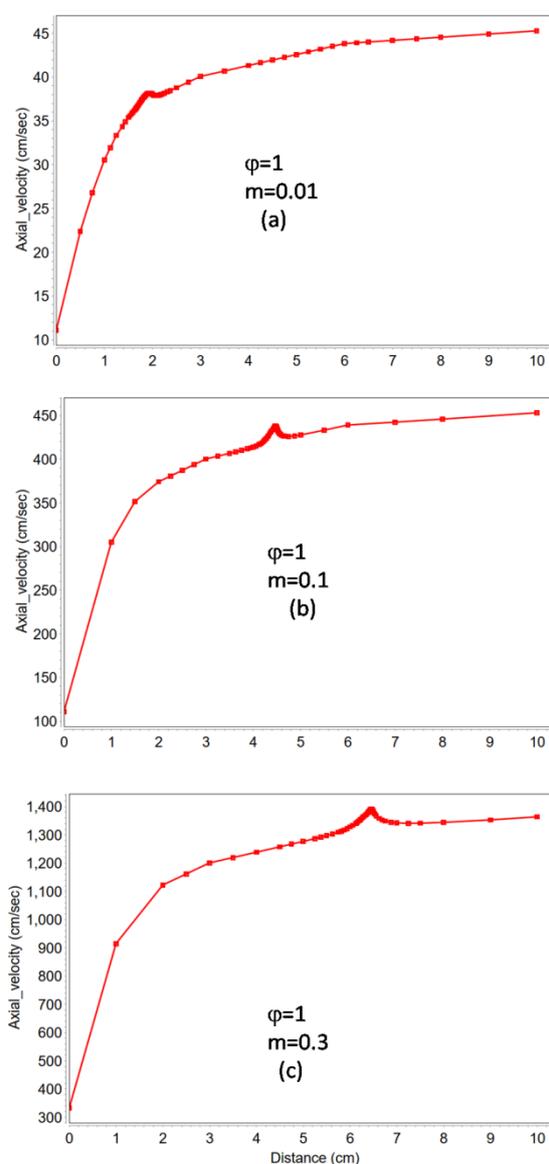


Figure 1. Axial velocity for stoichiometric CH₄+air a) $\dot{m}=0.01$, b) $\dot{m}=0.1$, c) $\dot{m}=0.3$ g/cm²s

In Figure 3 the mole fractions are given for mass flux of $0.1 \text{ g/cm}^2\text{s}$. These three figures are also drawn for lean, stoichiometric and rich mixtures combustion. As it is mentioned earlier the reaction occurs at a distance between 4 and 5 cm. As can be seen from Fig. 3.a. the products are the same as the ones in Fig.2.a. But the mole fractions of intermediates are higher for $\dot{m}=0.1 \text{ g/cm}^2\text{s}$ than the $\dot{m}=0.01 \text{ g/cm}^2\text{s}$. The values of mole fractions assume the same values for all of the mass flow rates.

The mole fractions in Fig.3.b are presented for the stoichiometric combustion of methane and air mixture at a mass flux of $0.1 \text{ g/cm}^2\text{s}$. Similar to the Fig.2.b. both methane and oxygen completely converted into the products. The mole fractions of the intermediates are higher than the ones in Fig.2.b.

The mole fractions for the rich mixture combustion at a mass flux of $0.1 \text{ g/cm}^2\text{s}$, are given in Fig.3.c. Similar to the Fig.2.c. reactants CH_4 and O_2 completely converted to the products H_2O , CO , CO_2 and H_2 .

For the mass flux of $0.3 \text{ g/cm}^2\text{s}$, mole fractions are presented in Figure 4. The reaction zone moves to the axial distance between 5 and 7.5cm from the inlet. Similar to the previous figures, Figure 4. is also presented for lean, stoichiometric and rich mixtures of methane and air. As can be seen from Fig. 4.a, there is O_2 at the product similar to the Fig.3.a and Fig.2.a. The mole fractions of the intermediates are higher than the ones at mass fluxes of $0.01 \text{ g/cm}^2\text{s}$ and $0.1 \text{ g/cm}^2\text{s}$. For the stoichiometric combustion, all the reactants are converted to the products as shown in Fig. 4.b. similar to the Fig.2.b and Fig.3.b. As can be seen from Fig.4.c, from reactants CH_4 and O_2 are

completely converted to the products H_2O , CO , CO_2 and H_2 . The mole fraction values of the products do not change with the mass flux.

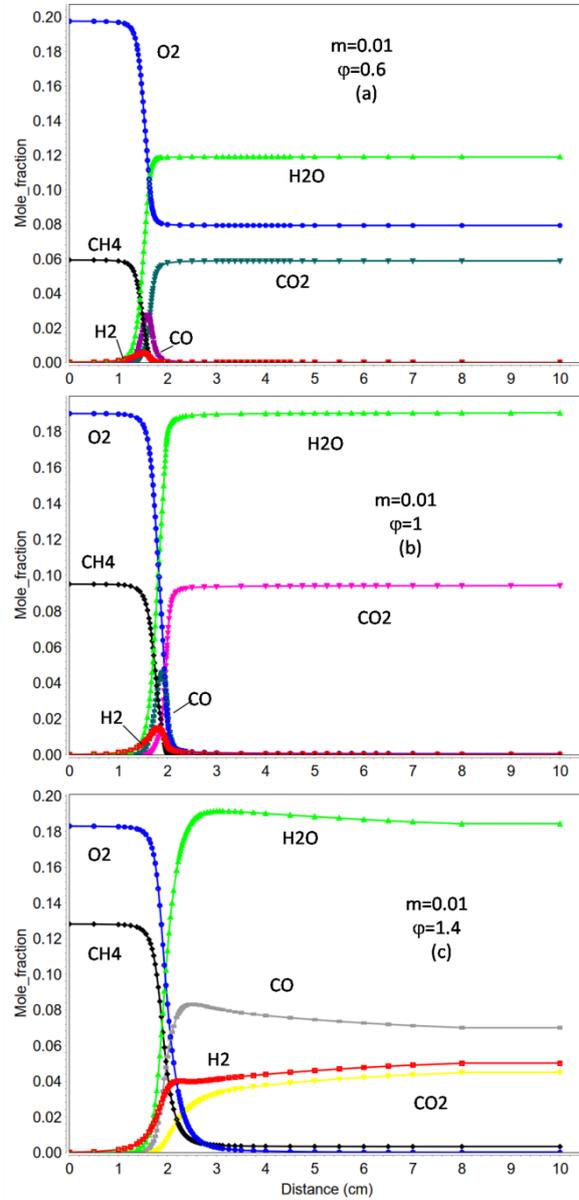


Figure 2. Mole fraction profiles of $\dot{m}=0.01$ a)lean b) stoichiometric c) rich mixture

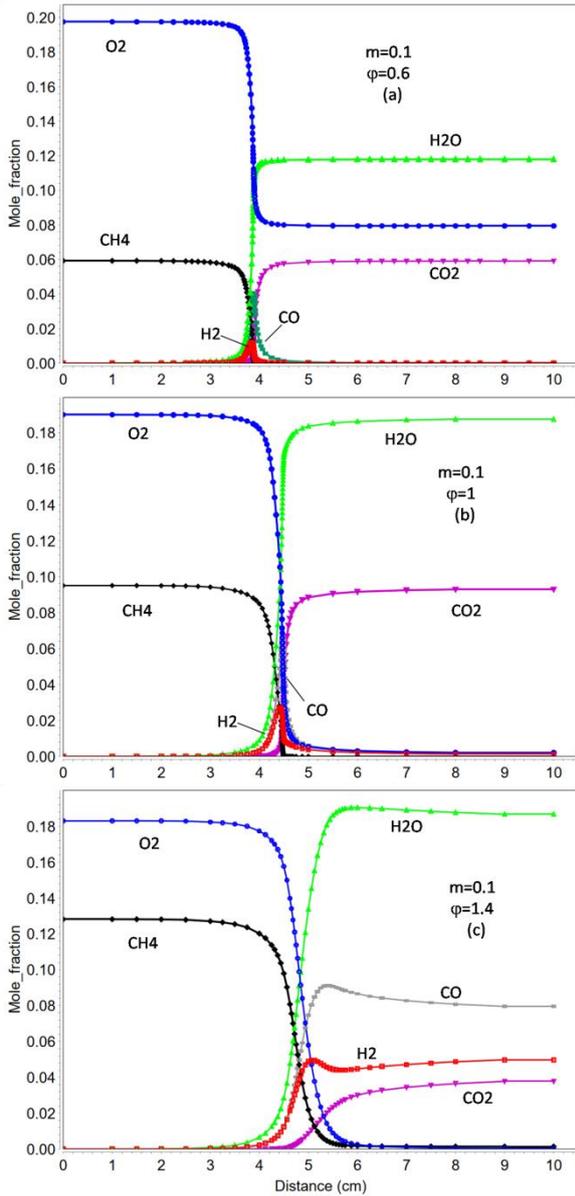


Figure 3. Mole fraction profiles of $\dot{m}=0.1$ a)lean b) stoichiometric c) rich mixture

4. Conclusion

In the present work one dimensional burner stabilized laminar premixes flame of methane and air is solved numerically by Chemkin 19 computer program with reaction mechanism GRI-Mech 3.0. The results are given as axial velocity and mole fractions for three different equivalence ratios (0.6, 1 and 1.4) and for three mass fluxes as 0.01, 0.1 and 0.3 g/cm²s

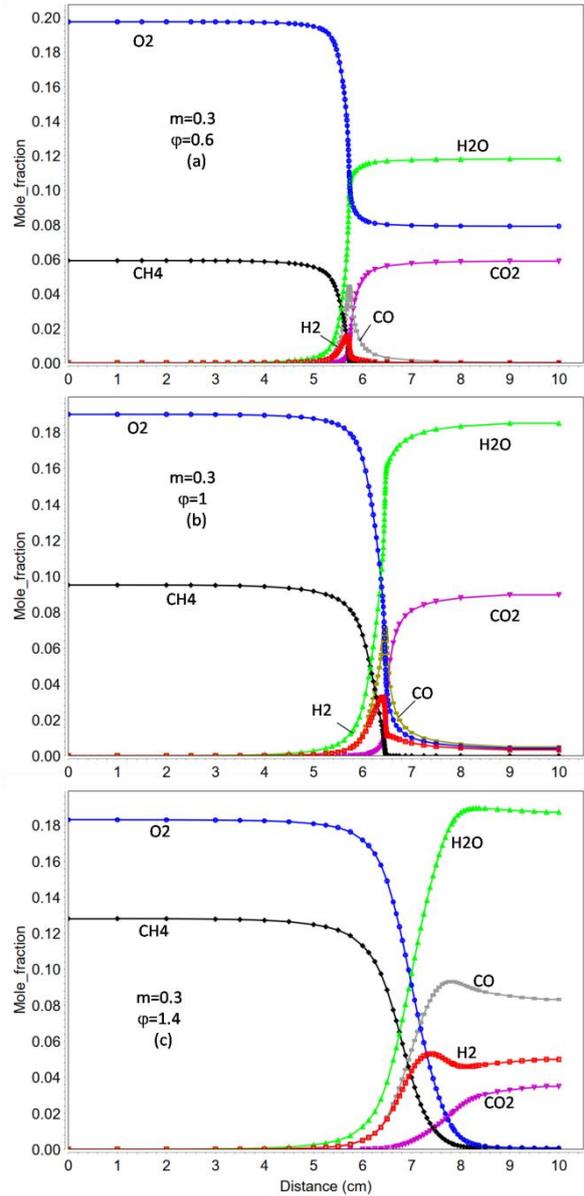


Figure 4. Mole fraction profiles of $\dot{m}=0.3$ a)lean, b) stoichiometric, c) rich mixture

The main results are as follows:

- With the increase of the mass flux, the axial velocities of the flame increases
- The axial location of the reaction zones increases with the mass flux.
- The mole fraction values of the intermediates increases with increasing mass flux.
- The mole fractions of the reactants are the same for all mass fluxes.

Acknowledgment

The author is grateful to Konya Technical University to ensure of ANSYS/Fluent CFD code.

Nomenclature

x	spatial coordinate
\dot{m}	mass flow rate
T	temperature
Y_k	mass fraction
k	index indicating the species
P	pressure
u	velocity of the fluid mixture
ρ	density
W_k	molecular weight of the k^{th} species
\bar{W}_{mean}	molecular weight of the mixture
R	universal gas constant
λ	thermal conductivity
c_p	specific heat of the mixture at constant pressure
c_{pk}	specific heat of the k^{th} species at constant pressure
$\dot{\omega}_k$	molar rate of production by chemical reaction of the k^{th} species per unit volume
h_k	specific enthalpy of the k^{th} species
V_k	diffusion velocity of the k^{th} species
\dot{Q}_{rad}	thermal radiation heat loss due to gas and particle
A	cross sectional area of the stream tube
X_k	mole fraction
D_{km}	mixture average diffusion coefficient
k_f	forward rate coefficient
V_c	correction velocity

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