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# Investigation of Methane-Air Laminar Flame to Apply in Internal Combustion Engines

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## Abstract

Even though combustion has been studied for a long time, however, due to complex essence of combustion which is a combination of different physical and chemical phenomena, there are still a lot of questions which should be addressed to improve efficiency of combustion systems such as internal combustion engines. Methane is one of the fuel which can be replaced to the normal fossil fuels such as gasoline and diesel. In this study laminar flame of a methane and air is studied in a freely propagating combustion tube. Different phenomena regarding to laminar flame such as laminar flame speed is studied. Subsequently, preheating zone, reaction zone and secondary reaction zone are studied and their thickness are reported. Finally, to understand the effect of operating conditions, parametric study of equivalence ratio and initial pressure are performed. Results showed that the laminar flame speed is maximum around the stoichiometric air and methane mixture. Also, with increasing the initial pressure, the laminar flame speed reduced monotonically.

**Keyword:** Methane, Combustion, Laminar Flame Speed, Free Propagating, Preheating and reaction zone, Secondary zone, Heat Release.

## 1. Introduction

What is known as natural gas is almost the chemical compound methane (95% or more) and the rest is longer carbon chains. Methane is an abundant fuel and after it is produced, it is can be compressed to a higher pressure or piped into different destination such as power plants, and factories for producing power or heat.

Due to less carbon hydrogen bonds in methane in comparison to other fossil fuels, methane combustion does not produce soot and it can be considered as a clean fuel. Therefore, there are a lot of studies which considered methane as a main source of energy in internal combustion engines [1-5]. The methane flame behaviors have been studied for various conditions [6–10]. Liu et al. [7] studied the chemical effects of methane combustion in CO<sub>2</sub> versus N<sub>2</sub>. Mazas et. al. [9] investigated numerically and experimentally, the laminar flame speed of mixture of methane and oxygen diluted with water and carbon dioxide. Mahabadipour et. al. [10] defined two new parameters based on second law of thermodynamics and reported theirs effects on different combustion zones such as flame zone and burned zone. Use of these parameter in our study helped us to compare the irreversibilities at different condition.

Study the effect of combustion systems on different phenomena such as combustion products can help to increase their efficiency. In fact, increasing the thermal efficiency of different combustion systems is one the main goal among researchers which motivated them to consider new combustion strategies or using different energy recovery system to utilize hot gas in the exhaust [11-15]. For example, Burch et. al. [12] investigated the effect of carbon dioxide and water on methane combustion over palladium catalyst.

In the current study, it is attempted to address the fundamental behavior of methane air combustion in a freely propagating combustion tube. Therefore, a mixture of air and methane in standard condition of 1 atm and 25 C is considered and effect of initial conditions such as pressure and equivalence ratio on laminar flame speed are reported.

## 2. Methodology

This simulation is used to determine the characteristic flame speed of the methane-air mixture at specified inlet temperature and pressure. In this study, heat losses are not considered and the energy equation can be invoked to compute the temperatures. Thus, the flame speed depends on the transport of energy (heat), and the temperature distribution prediction is a part of the flame speed calculation.

In this regard, freely propagating flame model for stoichiometric methane-air mixture at 25 C and 1 atm is studied using CHEMKIN-PRO. Therefore, the flame structure in terms of axial profiles of temperature, major species, and minor species, and heat release rate are investigated. The most recent version of GRI-MECH 3.0 kinetic mechanism [16] is applied in the model.

## 3. Governing Equations

1-dimensional flow with uniform inlet conditions is considered for solving the conservation equations (i.e., mass and energy) as well as equation of state and chemical kinetics equations [17]

Conservation of mass:

$$\dot{M} = \rho u A \quad (1)$$

Conservation of Energy:

$$\dot{M} \frac{dT}{dx} - \frac{1}{c_p} \frac{d}{dx} \left( \lambda A \frac{dT}{dx} \right) + \frac{A}{c_p} \sum_{k=1}^K \rho Y_k V_k c_{pk} \frac{dT}{dx} + \frac{A}{c_p} \sum_{k=1}^K \dot{\omega}_k h_k W_k + \frac{A}{c_p} \dot{Q}_{rad} = 0 \quad (2)$$

Species:

$$\dot{M} \frac{dY_k}{dx} + \frac{d}{dx}(\rho A Y_k V_k) - A \dot{\omega}_k W_k = 0 \quad (k = 1, \dots, K_g) \quad (3)$$

Equation of State:

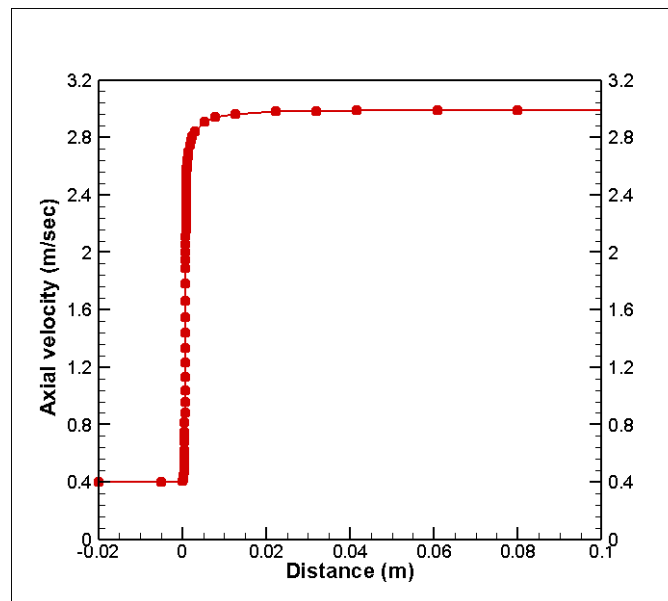
$$\rho = \frac{P \bar{W}}{RT} \quad (4)$$

Forward Chemical Kinetic Equation:

$$k_f = AT^\beta \exp\left(\frac{-E_A}{RT}\right) \quad (5)$$

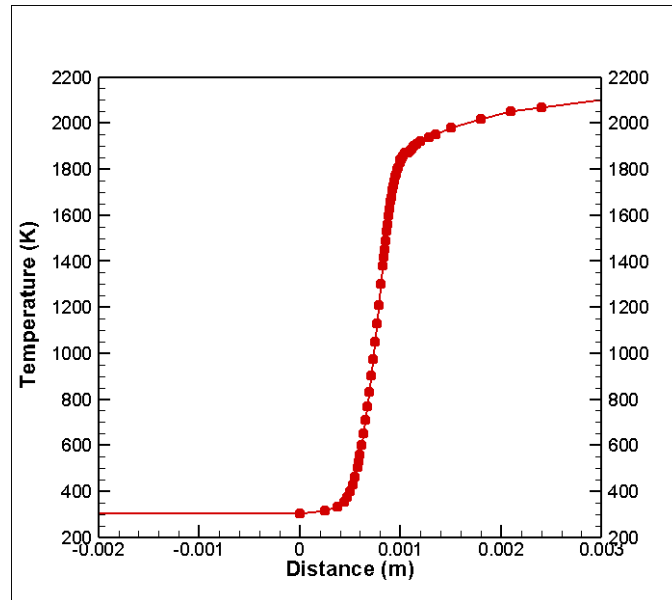
#### 4. Results and Discussion

In the following section, the results of methane air flame simulation are presented. The first parameter to discuss is laminar flame speed of mixture combustion. In Figure 1 it is shown that the laminar flame speed of mixture is 0.4 m/s which is compatible with other researchers results.



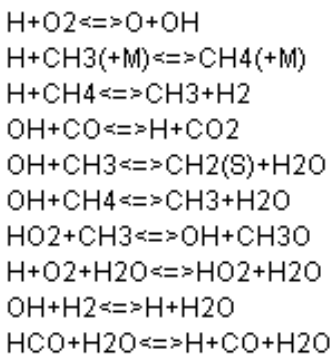
**Figure 1.** Axial velocity due to combustion of air and methane stoichiometric mixture

To identify the preheat zone and preheat zone thickness, temperature distribution of mixture along the combustion zone is reported. According to definition of the preheat zone, reactants are preheated to reach the ignition temperature.

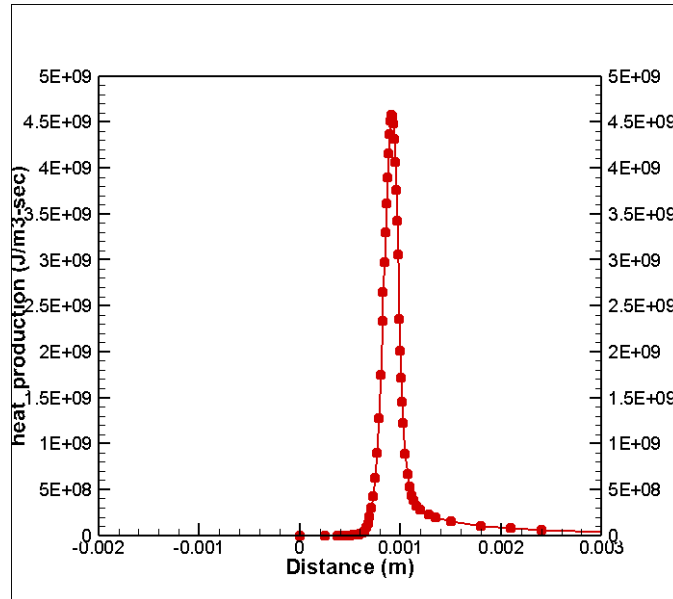


**Figure 2.** Temperature distribution due to combustion of air and methane stoichiometric mixture

Considering the auto ignition of methane which is around 810 K, it is found that the preheat zone reactants are preheated to reach the ignition temperature is around 0.0007 m (0.7 mm). Based on sensitivity analysis, in the preheating zone the following reactions are important:

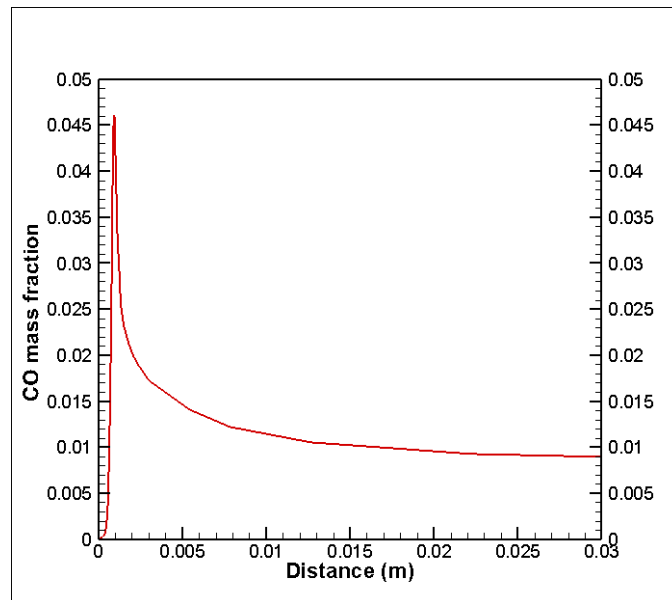


By knowing the thickness of preheat zone based on temperature distribution diagram, heat release curve can be used to identify the thickness of reaction zone. Based on heat release curve, reaction zone starts from 0.0007 m to 0.0012 m. Therefore, the reaction zone thickness will be 0.0005 m (0.5 mm)



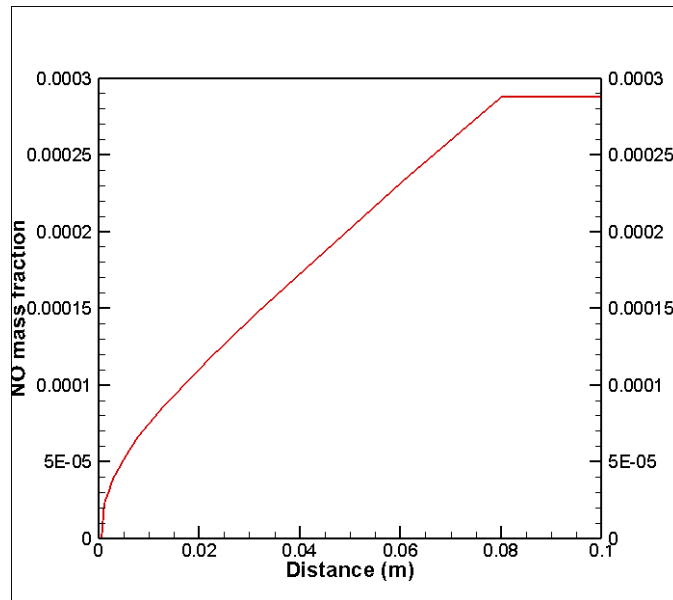
**Figure 3.** Heat release curve due to combustion of air and methane stoichiometric mixture

According to Figure 3, the post reaction zone occurs between 0.0012m to 0.015m which there is almost no heat release occurs, therefore, the length of secondary reaction zone is around 0.0014 m (1.4 mm). This result is compatible with the mass fraction of CO in the following figure:



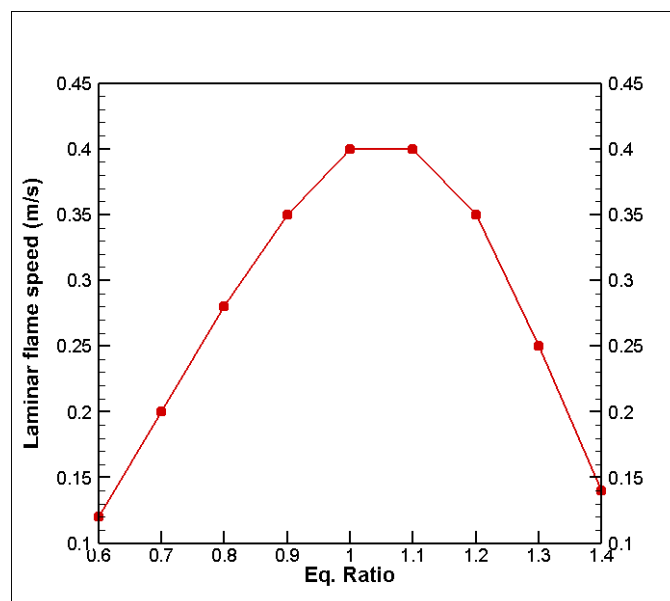
**Figure 4.** CO mass fraction due to combustion air and methane stoichiometric mixture

It is shown in Figure 5 that the most portion of NO is created in the secondary reaction zone. It might be due to rate of reaction of NO reactions which is slower than happening in the first reaction zone. Also, since most of heat release happens in the first reaction zone, therefore, N<sub>2</sub> can be dissociated after that in the post reaction zone and create NO.



**Figure 5.** NO mass fraction due to combustion air and methane stoichiometric mixture

A parametric study is conducted to compute the laminar flame speed versus equivalence ratio between 0.6 and 1.4 for methane-air mixture. The following figure shows laminar flame speed for different equivalence ratios:



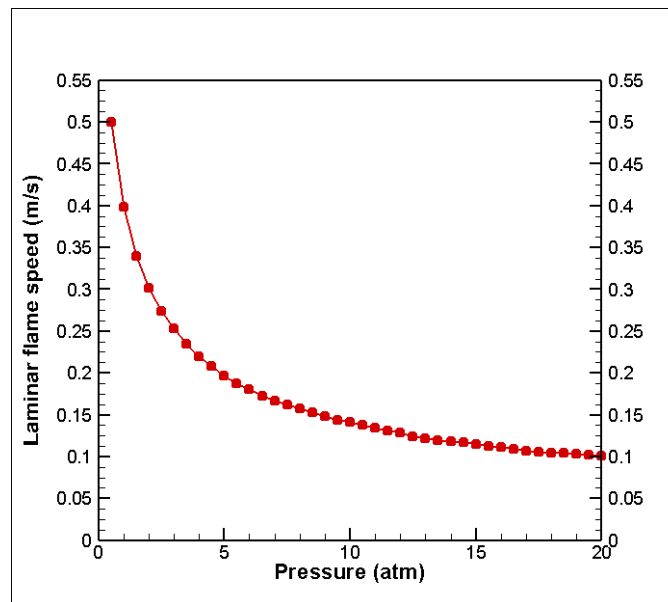
**Figure 6.** Laminar flame speed at different air and methane equivalence ratios

The results shown in Figure 6 are compatible with the experimental results of Ref [18]. It is represented that the maximum flame speed occurs around the stoichiometric mixture of methane and air. By reducing the equivalence ratio to a lean mixture (i.e. less than 1), the laminar flame speed reduced. The same results occurred for the rich combustion; with increasing the equivalence ration more than 1.1, the laminar flame speed reduced. According to laminar flame speed equation:

$$S_L = \left( \frac{T_{eq} - T_i}{T_i - T_o} \right) \frac{\alpha}{\delta_t} \quad (6)$$

Considering constant thermal diffusivity and flame speed, it is evident that with increasing equilibrium temperature, laminar flame speed increases. Therefore, since equilibrium temperature reaches its maximum at equivalence ratio around 1, its laminar flame speed reached the maximum too.

Finally, a parametric study for methane-air mixture is accomplished to compute and investigate the laminar flame speed versus pressure between 0.5 atm. and 20 atm. The results are shown in the following figure:



**Figure 7.** Laminar flame speed at different pressures

It is shown that with increasing the initial pressure, the laminar flame speed reduces, which might be due to reduction of equilibrium temperature. The results are compatible with the experimental results of Ref [19].



## **Summary and Conclusions**

In this study, laminar combustion of air and methane mixture in a freely propagating combustion tube was studied. In this regard, after reporting the governing equation, laminar flame speed was studied. Then, considering the heat release curve and combustion products, preheating zone, reaction zone and secondary reaction zone were studied and their thickness were reported. Finally, parametric study of equivalence ratio and initial pressure were performed and their effects on laminar flame speed were reported. Results showed that the laminar flame speed was maximum around the stoichiometric air and methane mixture. On the other hand, with increasing the initial pressure, the laminar flame speed reduced monotonically.

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