

# Effect of Hydrogen Addition to Methane Laminar Flames on Flame Speed and Pollutants

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## Abstract

This work presents the variation in the flame speed when both the hydrogen fraction in the incoming fuel and the equivalence ratio was varying. It has been found that the maximum flame speed shifts towards a richer side with an increase in the hydrogen content in the fuel. In addition to that, the influence of the presence of heat exchanger on NO<sub>x</sub> levels was investigated. Parameters such as the thermal conductivity and length of the heat exchanger were varied. The results revealed that the formation of NO is strongly related to temperature and the formation of NO<sub>2</sub> depends on the NO values. Also, cooling the flame in the reaction zone leads to the lowest NO<sub>x</sub> levels.

## Introduction

The world is moving towards renewable energy to reduce the dependency on fossil fuel usage in various sectors such as transportation, heating, and power generation to name a few. One of the main reasons behind this is to reduce the greenhouse gases emitted [1]. There is a growing interest in using hydrogen along with or instead of natural gas in practical combustion systems, such as gas turbines and domestic boilers since it can be produced with very little carbon emissions. However, this can cause various technical problems. This is currently an active area of research trying to solve those glitches. Gas-fired boilers are the current standard in heating the build environment. Hydrogen could play a major role in decarbonizing this sector. This paper is an early attempt in understanding the effect of the addition of hydrogen to methane fired boiler comprises of a burner and the heat exchanger. The results presented are generated using a 1-D flame simulation program called Chem 1-D, developed at Eindhoven University of Technology [2]. Two different flame configurations namely, free flame (adiabatic flame) and plug flow flame have been chosen. Variation in the flame speed is studied with the former using methane-hydrogen blend, while the latter was used to understand the impact of the heat exchanger on NO<sub>x</sub> emission using only hydrogen as a fuel.

## Simulation Setup

The details of the equation, modelling, and running a simulation can be found in reference [2]. Specific inputs have to be defined by the user according to the needs and flame type used. In this study, the equivalence ratio, inlet fuel composition and domain length were specified while using a free flame. In addition to the above, inlet mass flow has to be defined for plug flow flame. Once the heat exchanger has been added, the thermal conductivity, the length of the heat exchanger were defined to the program. Two chemical mechanisms such as GRI 3.0 [3] and NUI Galway [4] were used when the fuel is a methane-hydrogen blend and only hydrogen, respectively. All the

simulations were performed with an inlet temperature of 300 K and pressure of 1 bar. In this study, the methane fuel is substituted with hydrogen content varying from 10% to 100% (%v/v) with an interval of 10% is oxidized by air. The equivalence ratio has been varied from 0.6 to 1.3 with a step size of 0.1. These values were chosen to cover the wide range of operation for better understanding, although the practical boiler system prefers to operate with a fuel-leaner flame. The simulation setup is discussed in the next section followed by results and finishing with the main conclusions.

## Results and Discussions

The results are discussed in three parts. First, the variation of flame speed under different conditions are shown. Second, the investigation of NO<sub>x</sub> levels without a heat exchanger is presented and finally, the effect of the inclusion of heat exchanger on NO<sub>x</sub> levels is discussed.

### 1) Equivalence Ratio vs Flame Speed

The variation of unstretched adiabatic flame speed with the equivalence ratio is shown in Fig. 1. The flame

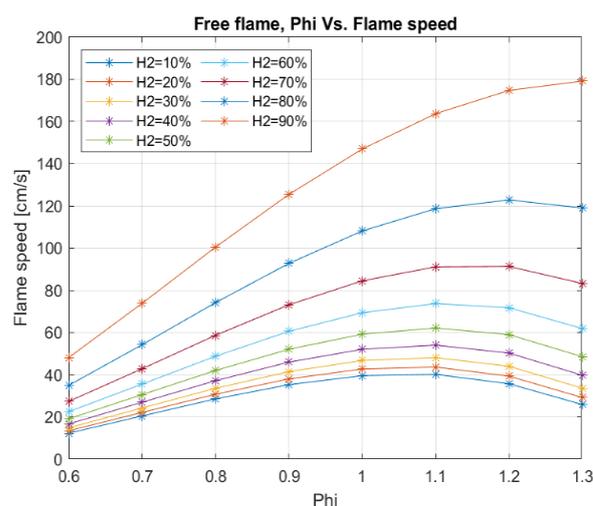
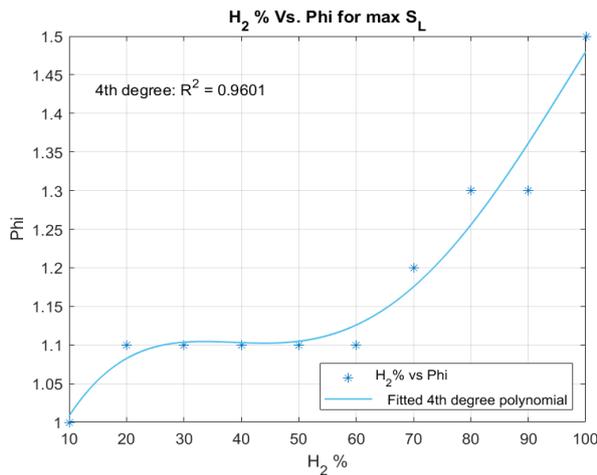


Fig. 1. Variation of flame speed with equivalence ratio at different hydrogen fractions.

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speed is calculated by dividing the mass flow at the last grid point by the density at the first grid point. It has been observed that the flame speed is sensitive to both the equivalence ratio and hydrogen fraction. It has been monotonically increasing with the increase in hydrogen fraction in the fuel at any equivalence ratio. However, the variation is much pronounced at hydrogen fractions greater than 40%. The Fig. 2 shows the equivalence ratios at which the maximum flame speed occurs at different hydrogen fraction. It was interesting to note that the equivalence ratio at which the maximum flame speed occurs, shifts towards the richer side with increasing hydrogen fraction in the incoming fuel stream i.e., the change is non-monotonic. A fourth degree polynomial curve has been fitted to the data points to qualitatively show the variation. At one end of the spectrum, pure methane at stoichiometric condition has a flame speed of 37 cm/s [5]. On the other end, pure hydrogen at stoichiometric condition can reach a flame speed of 150 cm/s. And, all the mixture has in-between values. So, when dealing with hydrogen and methane mixtures, a whole realm of flame speeds have to be handled in a careful way to design fuel flexible burners.



**Fig. 2.** Equivalence ratio for maximum flame speed at various hydrogen fractions.

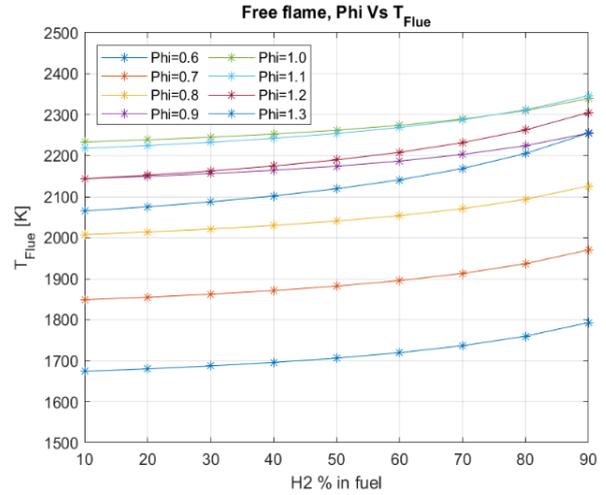
### 2) Variation of Adiabatic Flame Temperature

The variation of adiabatic flame temperature with both the equivalence ratio and hydrogen fraction is depicted in Fig. 3. It is clear that, unlike the flame speed, the adiabatic flame temperature is highly sensitive to equivalence ratio than to hydrogen level in the fuel. The variation of temperature across the equivalence ratio can go up to 30%. However, the maximum adiabatic flame temperature at various equivalence ratios will be achieved in the case with pure hydrogen as a fuel. Since NO<sub>x</sub> production is very sensitive to temperature [6], only pure hydrogen is considered in the following sections for explaining the NO<sub>x</sub> formation.

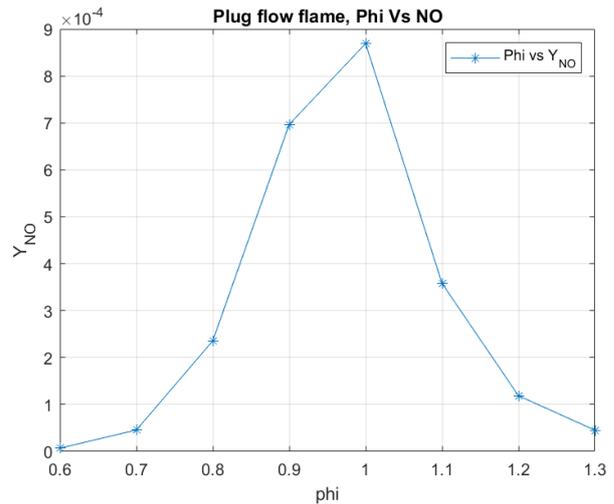
### 3) NO<sub>x</sub> Formation Without Heat Exchanger

In this section, the variation of NO and NO<sub>2</sub> with equivalence ratio and the relationship between NO and NO<sub>2</sub> formation and destruction is explained. The mass

fraction of the respective species at the last grid point is plotted against equivalence ratio for plug flow flame with pure hydrogen as a fuel is shown in Fig. 4 and Fig. 5.

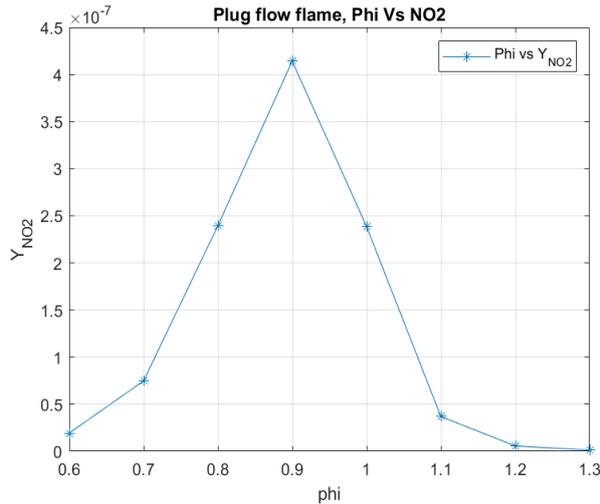


**Fig. 3.** Adiabatic flame temperature variation with hydrogen fraction at various equivalence ratios.



**Fig. 4.** Variation of mass fraction of NO with equivalence ratios

For NO and NO<sub>2</sub> to form, both the temperature and the oxygen radicals have to be present sufficient enough. Also, the formation of NO and NO<sub>2</sub> are related. It is explained as follows when the temperature is more than 1800 K, the nitrogen and oxygen react to form NO. When sufficient oxygen is available, the formed NO will be oxidized to NO<sub>2</sub>. However, when the temperature is high enough, the NO<sub>2</sub> splits back to NO and O. This goes on a cycle until an equilibrium is achieved. It is evident from the plots that when the NO level goes up, the NO<sub>2</sub> level falls. That is the reason behind the maximum NO occurs at an equivalence ratio of 1 whereas the maximum NO<sub>2</sub> occurs at an equivalence ratio of 0.9. On the richer side, even though the temperature is greater than 1800 K, the absence of sufficient oxygen radicals prevents the formation of NO and also, inhibits the oxidation of NO to NO<sub>2</sub>.

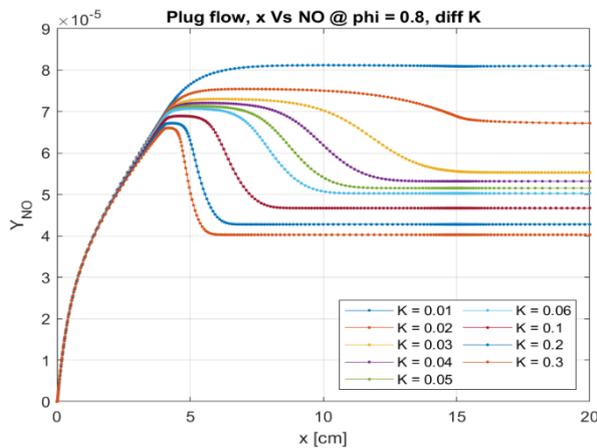


**Fig. 5.** Variation of mass fraction of NO<sub>2</sub> with equivalence ratios.

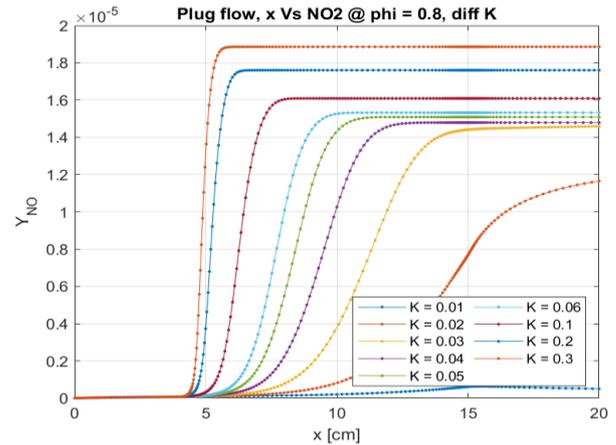
4) *Effect of Heat Exchanger on NO<sub>x</sub> - Variable Thermal Conductivity (K):*

To understand the effect of cooling the flame on NO<sub>x</sub> emission, a 1-D heat exchanger has been added to the plug flow simulation. The heat exchanger acts as a heat sink at a constant temperature. The properties of the heat exchanger such as its thermal conductivity and length were varied. The length of the heat exchanger is varied by adjusting the starting position while the end position is fixed.

In this case the heat exchanger length and the temperature at which the heat exchanger present were fixed while only the values of thermal conductivity were varied. The heat exchanger fixed at 400 K, starts at 4 cm and ends at 15 cm across the domain length of 20 cm. The variation of NO and NO<sub>2</sub> across the domain at an equivalence ratio of 0.8 for various thermal conductivity is shown in Fig. 6 and Fig. 7, respectively. By adjusting the thermal conductivity, the rate of cooling can be adjusted. So, at higher K values, (K = 0.1, 0.2, 0.3 W/m.K) sudden drop in temperature of the flame as opposed to a gradual drop as in the case of low K values has been observed as expected.



**Fig. 6.** Variation in mass fraction of NO at equivalence ratio of 0.8 for different thermal conductivity.

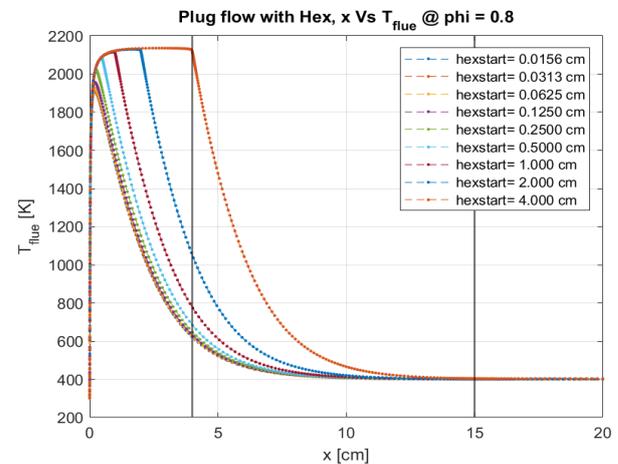


**Fig. 7.** Variation of mass fraction of NO<sub>2</sub> at equivalence ratio of 0.8 for various thermal conductivity.

From the plots, it has been observed that, as the flame cools while encountering the heat exchanger, the temperature drop causes the NO values to drop. In some cases, even though the temperature drops, the NO remains the same since the temperature the flame has been cooled to is still enough for the already formed NO to sustain. As explained earlier, the formation of NO<sub>2</sub> is strongly related to NO as can be observed from the plot, when the value of NO drops, NO<sub>2</sub> begins to rise. This is because, as the temperature of the flame has been reduced, which prohibits the conversion of NO<sub>2</sub> to NO and O. This effect is more pronounced when the cooling is drastic as in the cases of the heat exchanger with high K values.

5) *Effect of Heat Exchanger on NO<sub>x</sub> – Variable cooling location:*

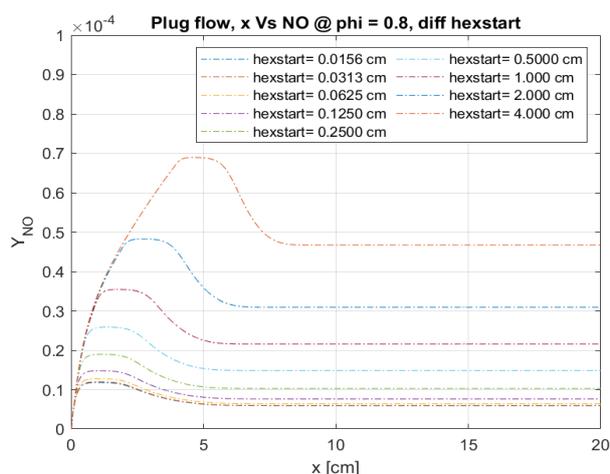
In the earlier section, the length (in turn position) of the heat exchanger is fixed. However, it is intriguing to study the effect on NO<sub>x</sub> evolution of starting position from where the flame is being cooled. The procedure of moving the heat exchanger starting point closer to the flame while the ending point of the heat exchanger is



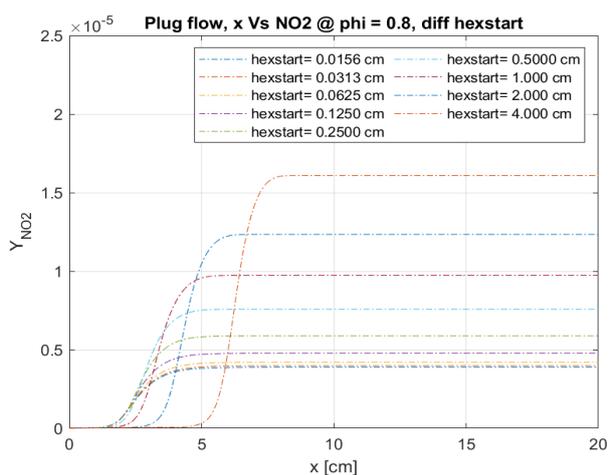
**Fig. 8.** Temperature profile when the heat exchanger starting position is varied.

fixed at 15 cm is followed. In this way, the length of the heat exchanger is changed. The thermal conductivity and temperature of the heat exchanger are fixed at 0.1 W/m.K and 400 K, respectively. Since the thermal conductivity at which the heat exchanger presents is enough for cooling the flame to the temperature of the heat exchanger irrespective of the starting of the cooling position. The temperature profile is shown in Fig. 8. The two solid lines at 4 cm and 15 cm are the reference lines to compare the temperature profile with other cases.

The change in the position of cooling resulted altogether in a different picture on  $\text{NO}_x$  evolution. The variation of NO and  $\text{NO}_2$  across the domain at an equivalence ratio of 0.8 is shown in Fig. 9 and Fig. 10, respectively.



**Fig. 9.** Variation in mass fraction of NO at equivalence ratio of 0.8 for different heat exchanger starting position.



**Fig. 10.** Variation in mass fraction of  $\text{NO}_2$  at equivalence ratio of 0.8 for different heat exchanger starting position.

When the temperature of the flame cools to the temperature of the heat exchanger, the NO does not drop to zero even though the temperature is less than the temperature needed for NO to form (i.e., more than 1800

K). The position of cooling controls the formation of NO as seen in the plot. If the flame has been cooled at a faraway position, enough NO has been already formed which will survive this drastic temperature change. From Fig. 10, it is interesting to note that, cooling the flame very near or inside the reaction zone leads to less  $\text{NO}_2$  because, the NO has been formed is very low and there is not enough temperature to cause the dissociation of  $\text{NO}_2$  to NO and O. As expected, there is an increase in  $\text{NO}_2$  whenever there is a fall in NO levels. However, cooling the flame very near or inside the reaction zone leads to very low NO and  $\text{NO}_2$  levels compared to cooling the flame further downstream.

## Conclusions

A preliminary attempt has been made in understanding the changes in flame speed while using a hydrogen-methane blend at various equivalence ratio and hydrogen fraction in the incoming fuel.  $\text{NO}_x$  emission characteristics with and without the heat exchanger have also been conducted by using pure hydrogen as a fuel. The important conclusions are as follows:

- The flame speed is sensitive to both hydrogen fraction in the inlet and equivalence ratio.
- A shift in peak flame speed moves towards the richer side with an increase in hydrogen fraction.
- Adiabatic flame temperature is sensitive to equivalence ratio only.
- The formation of NO and  $\text{NO}_2$  requires both temperature and oxygen-free radicals. Also, the formation of NO and  $\text{NO}_2$  are related.
- Cooling the flame can lead to lesser  $\text{NO}_x$  levels. However, the cooling position may have an impact on them.
- It has been observed that cooling the flame near or inside the reaction zone leads to the least NO and  $\text{NO}_2$  levels.

These results are all preliminary and have to be confirmed with experiments and higher dimensional simulations. The building of experimental setup and performing numerical simulations are in progress.

## Acknowledgements



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