

COMPUTATION OF LAMINAR HYDROGEN FLAMES

Piotr Pasiak



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Piotr Pasiak

Department of Mechanical- and Marine Engineering

Western Norway University of Applied Sciences

NO-5063 Bergen, Norway

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Høgskulen på Vestlandet

Fakultet for Ingeniør- og Naturvitenskap

Institutt for maskin- og marinfag

Inndalsveien 28

NO-5063 Bergen, Norge

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Piotr Pasiak, 584415

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Contact person: Shokri Amzin

Preface

This bachelor thesis is written at the Department of Mechanical and Marine Engineering at Western University of Applied Sciences (WNUAS) and in the General Mechanical Engineering study. Project supervisor is Dr Shokri Amzin, his primary research focuses is directly on understanding of practical applications and the environmental impact of energy conversion. Primary the zero-emission energy and energy systems.

Abstract

The increase of the overall energy consumption in the world results in higher greenhouse gas emissions and an increase in global temperature. Lean premixed combustion of hydrogen is one of the most promising methods to replace hydrocarbon fuels and reduce emissions whilst maintaining high efficiency in combustion systems. As the consequences of global warming are more visible, modelling of laminar hydrogen-air premixed combustion is becoming an important tool for designing environmentally friendly and efficient alternatives for combustion systems. In order to move forward and replace fossil-based energy sources with renewable and efficient green methods predictive and reliable models are required. One of the methods is Chemical Kinetics used to perform numerical computations for chemical reactions. In this study numerical computations on laminar hydrogen flame are performed using chemical kinetics and a software called Cantera. The aim is to present one of many options on how models for a combustion system can be constructed and what parameters of the chemical reaction can be investigated in order to achieve a reliable model. The chemical reaction in this study is a laminar premixed hydrogen-air combustion at different initial pressure and temperature. Parameters like laminar flame speed S_L^0 , flame temperature, mass fraction of species and heat release rate in the reaction are investigated. Other results important for creating a reliable model are presented for different initial values.

Sammendrag

En økende forbruk av energi i verden fører til at mengden drivhusgasser i atmosfæren blir større og den globale temperaturen vokser. Mager forblandet forbrenning av hydrogen er den mest lovende erstatningen for hydrokarbonbrensel og reduksjon av utslipp samtidig som den høye effektiviteten i forbrenningssystemer beholdes. Nå som konsekvenser av globaloppvarming blir mer og mer synlige, er generering av laminær hydrogen-luft forblandet forbrenning enda mer viktig redskap for å lage miljøvennlige og effektive modeller av forbrenningssystemer. For å gå videre og erstatte fossile energikilder med fornybare og effektive grønne metoder, trenges det pålitelige og forutsigbare modeller. En av sånne metoder er kjemisk kinetikk som er brukt til å utføre numeriske beregninger av kjemiske reaksjoner. I denne forskningen er det utført numeriske beregninger på laminær hydrogenflamme ved hjelp av kjemisk kinetikk og program kalt Cantera. Målet med denne forskningen er å presentere en av mange mulige metoder for hvordan modeller for forbrenningssystemer kan bli konstruert og hvilke parametere av kjemisk reaksjon kan bli undersøkt for å lage pålitelige modeller. Den kjemiske reaksjon undersøkt i denne forskningen er laminære forblandet hydrogen-luft forbrenning for forskjellig start trykk og/eller temperatur. Verdier som for eksempel laminær flammehastighet S_L^0 , flammetemperatur, massefraksjon av forskjellige stoffer og varmeutslippshastighet er undersøkt. Andre resultater for viktige parametere nødvendige for generering av pålitelige modeller er også presentert for forskjellige start verdier.

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1. Introduction

The development in technology and production methods allows more people access to better technology and worldwide travel which increases the overall energy consumption. Unfortunately, the main source of energy in the world today is combustible carbon-based fuels like petrol and coal due to their high energy density and availability. The oxidation of these hydrocarbons contributes to the increase of greenhouse gases and disturbs the natural carbon cycle in earth's atmosphere. Climate change is one of the biggest threats of our time, not only because of the drastic environmental changes, but also the health and economic issues. Thus, it is important to reduce and/or totally exchange hydrocarbons with low and zero emission fuels such as natural gas and hydrogen.

Hydrogen-air combustion is one of the best options to consider for future transportation and power generation applications because of its high efficiency. As a mixture they emit far fewer emissions than non-renewable fuels. Hydrogen gas can be generated from the excess energy produced from renewable sources such as wind and solar energy. This will make the carbon footprint of hydrogen zero. Particularly, when it is burned in Lean Premixed Combustion (LPC) (more air and less fuel). However, utilising lean premixed to industrial combustors is not straightforward due to its thermoacoustic instability, and hydrogens increase of the enigma complexity. Performing physical test and research on combustion can be very expensive and require big and expensive machines, therefore it is equally important to perform numerical computations and develop models to understand physics and chemistry of the reaction.

In order to move forward reliable and predictable models for the chemical reaction are necessary. These models will serve as a tool in development of low and zero emission combustion systems. The model can also be used to investigate the combustion characteristics of other gas mixtures or renewable

fuels of interest. In this study chemical kinetics and software called Cantera is used to perform numerical calculation on laminar premixed hydrogen-air combustion. Results like laminar flame speed S_L^0 , flame temperature, mass fraction of species and heat release rate in the reaction are investigated and presented and investigated for different initial pressures. The aim is to present one of many options of how chemical kinetics can be used to obtain important parameters needed to create such models.

2. Background

Combustion is a chemical reaction between reactants, fuel, and oxidiser. The reaction produces heat and light in form of flame. Usually, the rate at which the reactants combine is high, this is in part because the energy produced is much higher than the rate at which it can escape into the surrounding medium. This causes the temperature to rise and accelerate the reaction even more. It can be categorized as being either premixed or non-premixed flames. A high percentage of the electricity produced in the world comes from the combustion. This study of Laminar Hydrogen Flames is important because it contributes to the reduction of pollutants released into the atmosphere.

Some key parameters for this study are:

- ϕ , Equivalent ratio:

Is the ratio between substances in a given chemical reaction normalized by the stoichiometric ratio.

Given by formula:

$$\phi = \frac{\frac{n_{air}}{n_{fuel_{actual}}}}{\frac{n_{air}}{n_{fuel_{stoich}}}}, \quad n = \text{massfraction or number of moles}$$

Figure 1 shows the equivalence ratio plotted against the flame speed for laminar premixed combustion of paraffine. When the equivalence ratio ϕ is 1, it means that the mixture of fuel and oxidiser is stoichiometric, and the reaction will be complete. If the $\phi > 1$, it means that the fuel/oxidizer ratio is bigger than the stoichiometric and the amount of fuel is higher than that of the stoichiometric. The excess of fuel is also called Rich Mixture. For $\phi < 1$, the fuel/oxidant ratio is

smaller than that the stoichiometric and the amount of fuel is lower.
Having excess of air is called Lean Mixture.

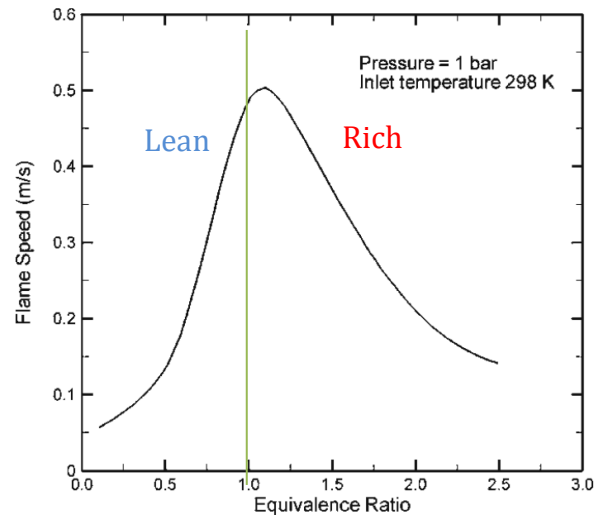


Figure 1 - Laminar premixed paraffin combustion,
flame speed vs equivalence ratio (12)

- S_L^0 , Laminar Flame Velocity:

Plays a key role in understanding premixed combustible mixture's reactivity, diffusivity and the exothermicity. It is the speed that the unstretched laminar flame propagates relative to the unburned mixture. The fuel/oxidiser enters the system at the unburnt velocity v_g . S_L^0 is the velocity at which the flame front propagates in the unburnt mixture. For the flame to remain fixed in an exact position the S_L^0 must equal v_g .

2.1 Theoretical approach

2.1.1 Premixed and Non-Premixed Flames

Premixed combustion means that the fuel and oxidizer are mixed before they reach the reaction zone. In this case the reaction zone is defined by balancing the local collective velocity of the fuel-oxidiser mixture with the rate at which the reactants are consumed. This is different to the non-premixed combustion where the fuel and the oxidiser reaches the reaction zone unmixed. In such case the reaction zone is defined in the location where the total enthalpy of the reactants balances out with the product of the reaction and the energy losses. The non-premixed reaction ideally takes place at stoichiometric conditions. This usually gives the maximum flame temperature for given fuel-oxidiser mixture. For the premixed combustion based on the stabilizing method, the reaction can take place at equivalent ratio other than 1. This can give a lower flame temperature.

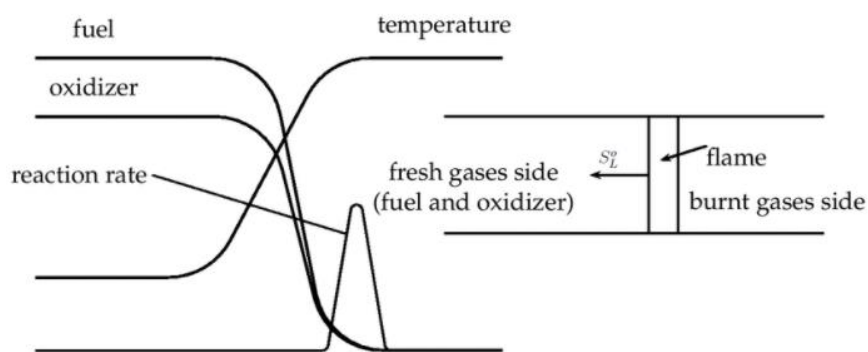


Figure 2 - Structure of a laminar premixed flame (13)

Figure 2 shows the combustion mode for the laminar premixed flame. As the figure above represents the oxidiser and the flame are mixed before the reaction begins. At the point of the reaction the temperature is rapidly increased. This is opposite to the non-premixed combustion where at the end of the reaction the temperature is much lower. Also, the reaction rate reaches the maximum when almost all the reactants have been consumed.

2.1.2 Laminar Premixed Flame

Most of the combustion processes are turbulent, but most of them are based on laminar processes and can therefore be described by its equations.

2.1.3 Transport Equations

- Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0$$

Mass conservation law states that the total increase of the mass of species in a Control Volume (CV) is equal to the net mass flow into the CV plus the species formation rate in the CV.

- Conservation of momentum:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = - \frac{\partial \rho}{\partial x_i} + \frac{\partial(\tau_{ij})}{\partial x_j} + F_i$$

The law of conservation of momentum is Newton's second law applied for Fluid Mechanics. It means that the change of the total momentum in a CV plus the exchange of the momentum with outside of the CV equal to the force acting on the boundary of CV plus the body force on the CV.

- Conservation of mass fraction species of α :

$$\frac{\partial(\rho Y_\alpha)}{\partial t} + \frac{(\rho u_i Y_\alpha)}{\partial x_i} = - \frac{\partial J_i^\alpha}{\partial x_i} + \dot{\omega} \quad (\alpha = 1, 2, 3, \dots, N)$$

This equation represents on the left-hand side the local rate of change of Y_α and the convective transport. And on the right-hand side the molecular diffusion flux of species α in the i 'th direction and the total rate at which the mass is produced in the chemical reaction.

- Conservation of energy:

$$h = \sum_{\alpha=1}^n Y_\alpha h_\alpha$$

Where h is the enthalpy of a reactive mixture.

$$h_\alpha = h_{f_\alpha}^0 + h_s^s$$

h_α is the enthalpy for species α . The equation above shows that the species enthalpy equals to the sum of the formation enthalpy and the enthalpy of species α at sensible enthalpy and reference temperature.

The sensible enthalpy h^s for an ideal gas is given as:

$$h_\alpha^s = \int_{T_{ref}}^T C_{p\alpha}(T) dT$$

The equation for conservation can also be simplified assuming the Low Mach number flow to:

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial(\rho u_i h)}{\partial x_i} = \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} \left(\frac{\lambda}{C_p} \frac{\partial h}{\partial x_i} \right) + S_R$$

Where the left-hand side of the equation is the local temporal change of ρh and the convective transport inside a CV. The right-hand side of the equation is the pressure gradient, the diffusion of the enthalpy and the sink term because of radiative heat exchange.

- State equation:

$$p = \rho RT \sum_{\alpha=1}^n \frac{Y_{\alpha}}{W_{\alpha}}$$

Where the pressure p , is derived from this state equation.

- Progress variable:

In premixed combustion, the progress variable C is used to quantify the reaction progress using the temperature T and the fuel mass fraction Y_f .

$$C_T = \frac{T - T_u}{T_b - T_u}, \quad \text{or} \quad C_f = \frac{Y_f - Y_f^u}{Y_f^b - Y_f^u}$$

Terms T_u, Y_f^u and T_b, Y_f^b represent the temperature and the fuel mass fraction of unburnt and burn mixture in adiabatic flames.

One can also use the sensible enthalpy, which gives the equation:

$$c = \frac{h^s - h_u^s}{h_b^s - h_u^s}$$

This gives:

$$\frac{\partial(\rho c)}{\partial t} + \frac{\partial(\rho u_i c)}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\rho D_c \frac{\partial c}{\partial x_i} \right) = \rho \dot{\omega}_c$$

- Mixture fraction:

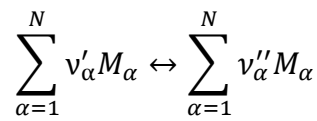
The mixture fraction Z describes the mass fraction of the reacting mixture. It is normalized such that it approaches one in the fuel stream and zero in the oxidiser stream.

The instantaneous transport equation is given by:

$$\frac{\partial(\rho Z)}{\partial t} + \frac{\partial(\rho u_i Z)}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\rho D_z \frac{\partial Z}{\partial x_i} \right) = 0$$

- Reaction rates:

Is the speed at which a chemical reaction takes place. An I elementary reaction can be expressed in a symbolic form:



The k , net rate of chemical reaction is given by:

$$\dot{\omega}_k = k_{fk} \prod_{\alpha=1}^N \left(\frac{\rho Y_{\alpha}}{W_{\alpha}} \right)^{v'_{\alpha k}} - k_{bk} \prod_{\alpha=1}^N \left(\frac{\rho Y_{\alpha}}{W_{\alpha}} \right)^{v''_{\alpha k}}$$

Where the k_{fk} and k_{bk} represent forward and backward rate coefficients, W_{α} represents the molecular weight of species α and the $v'_{\alpha k}$ and $v''_{\alpha k}$ represent the forward and backward stoichiometric coefficients.

The k coefficient can be described by:

$$k = AT^n e^{-\frac{E_a}{RT}}$$

Where the E_a is the activation energy and A is the pre-exponential factor.

This gives the expression for the chemical reaction rate for species α , given mass:

$$\dot{\omega}_{\alpha} = W_{\alpha} \sum_{k=1}^I \dot{\omega}_k (v''_{\alpha k} - v'_{\alpha k})$$

2.1.4 Combustion of Hydrogen

One of many differences between combusting hydrogen and fossil fuels is the wide flammability range of hydrogen. Hydrogen can combust in a wide range of fuel-air mixture. This means that the hydrogen can run on a lean mixture which results in a greater fuel economy and generally a lower final combustion temperature.

Hydrogen has also a greater auto-ignition temperature. This enables a higher compression ratio than regular fossil fuel. A higher compression ratio results in greater thermal efficiency, which means lower energy losses during combustion.

One other advantage of using hydrogen as fuel rather than carbon-based fuels is the products from the combustion. Burning hydrogen in air produces water, making the hydrogen fuel a carbon neutral replacement for fossil fuels.

2.1.5 Limitations

As the wide flammability range is an advantage, it can also be a disadvantage. The wide flammability range of hydrogen makes it dangerous because of the unpredictability. It makes it harder to control the combustion in the same way as for hydrocarbon engines.

2.2 Method

2.2.1 Chemical Kinetics

Chemical kinetics is a branch of physical chemistry that focuses on understanding the rates of chemical reactions. It includes the study of how experimental conditions can affect the rate at which a chemical reaction happens and give insights into the reaction's mechanism and transition states. Chemical kinetics is also used to construct mathematical models that can be used to describe characteristics of a chemical reaction.

2.2.2 Cantera

Cantera is an open-source software developed to solve problems involving chemical kinetics, thermodynamics, and transport processes. In this study it is used for solving chemically reacting laminar flows. It was originally written and developed by Prof. Dave Goodwin of California Institute of Technology. The software is written in C++ and it can be used from C++, MatLab, Fortran and Python. Python being the language used for this study. Cantera is used to help solve complex chemical kinetics problems. It allows a more efficient investigation of potentially new problems compared to direct experimental investigation. The software produces simulations of freely-propagating, premixed flat flames for a given kinetic mechanism and initial Temperature, pressure and composition conditions.

2.2.3 Software

The software Cantera is used through an Integrated Development Environment (IDE) called Spyder. The IDE is used to specify ϕ , equivalence ratio, initial temperature, and pressure. The laminar flame velocity S_L^0 and

maximum temperature are than plotted with respect to the equivalence ratio.
A MatLab script and Excel is than used to evaluate results generated in Spyder.

3. Results

3.1 Laminar flame velocity S_L^0 :

The first thing calculated is the Laminar Flame Velocity S_L^0 . Figure 3 shows S_L^0 for pressures 0.5, 1, 2, 3 and 5 times the atmospheric pressure vs the Equivalence ratio ϕ on x-axis.

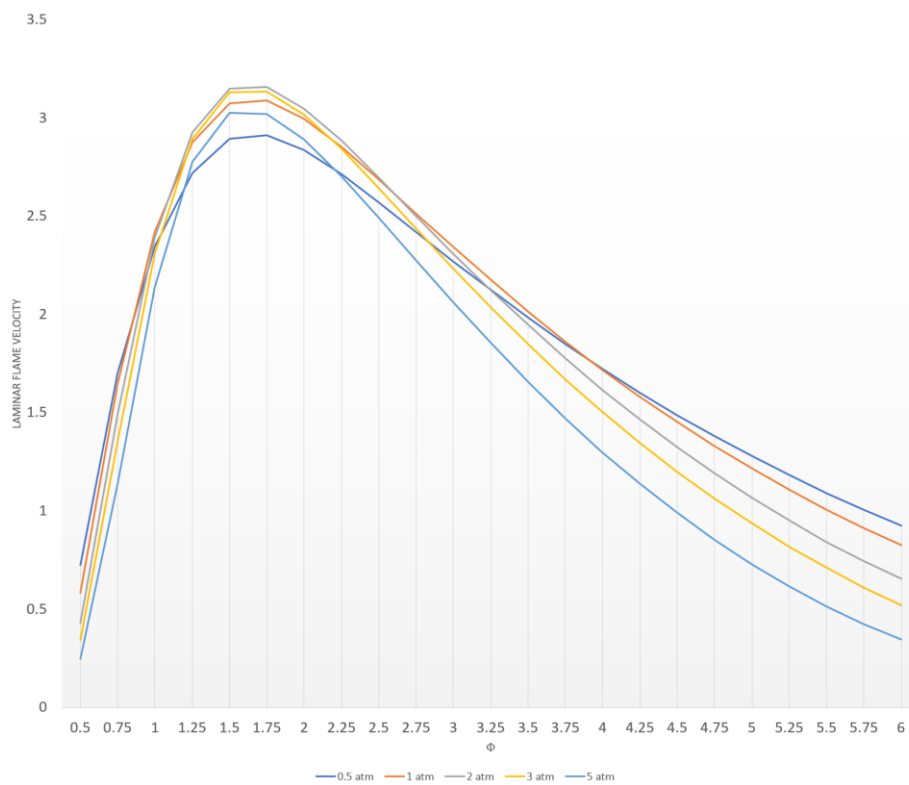


Figure 3 - Laminar Flame Velocity for different pressures.

The S_L^0 is the highest at around 1.5 – 1.75 ϕ . It reaches 3.15 m/s for 2 times the atmospheric pressure and is the lowest for 0.5 atmospheric pressure at 2.9 m/s. This means that combusting hydrogen in air at two times the atmospheric pressures is most efficient.

3.2 Flame Temperature

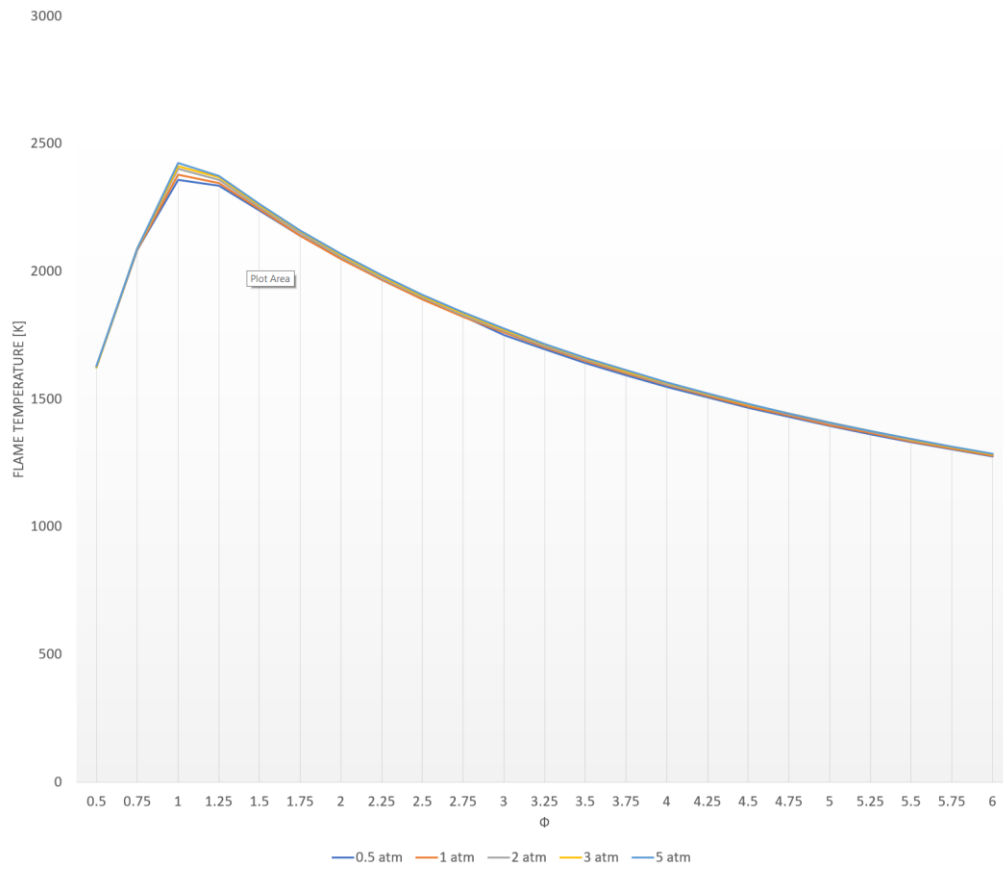


Figure 4 - Flame temperature for different pressures

The Flame temperature is compared for different pressures. Figure 4 shows that the temperature is at its maximum for equivalence ratio $\phi = 1.25$. It also shows that the maximum temperature increases slightly with the pressure.

3.3 Mass Fraction of Species

The figures below (Figure 5, Figure 6 and Figure 7) show the mass fraction of O_2 , H_2O and H_2 at different spatial coordinates of the combustion.

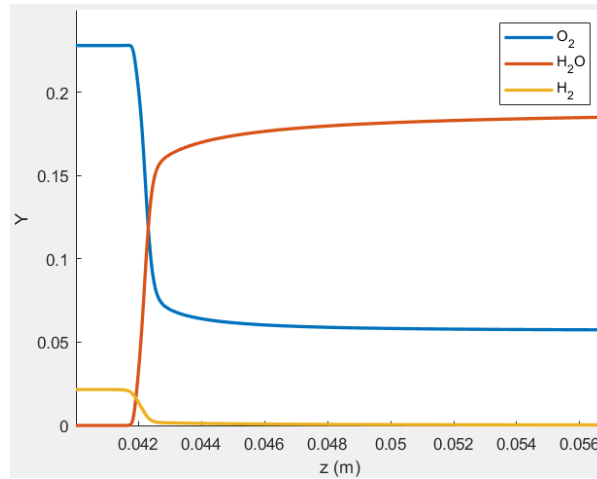


Figure 5 - Mass Fraction of different species for Phi = 0.75, P=0.5 atm

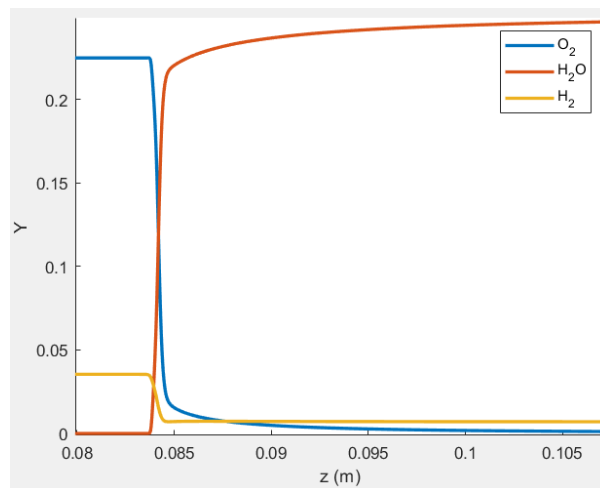


Figure 6 - Mass Fraction of different species for Phi = 1.25, P=0.5atm

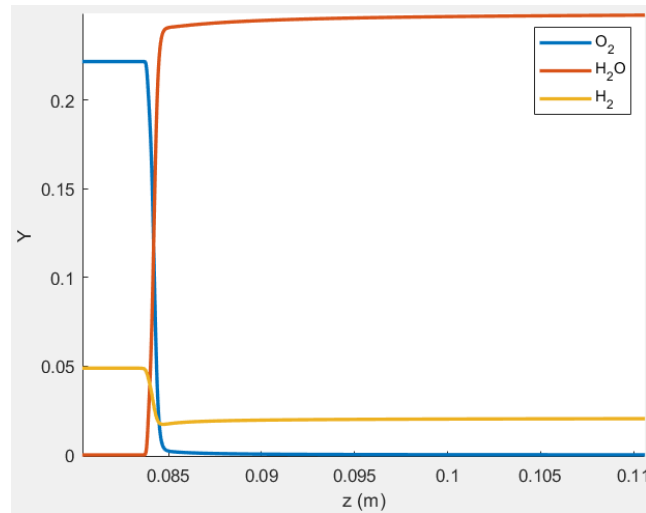


Figure 7 - Mass Fraction of different species for $\Phi = 1.75$, $P=0.5\text{atm}$

These plots show that the reaction zone is different for the lowest equivalence ratio of $\phi = 0.75$. It also shows that the highest temperature is a result of more of the mixture contributing to the reaction. As shown in previous section the laminar flame velocity S_L^0 is highest when the equivalence ratio $\phi = 1.75$, but from the Figure 7 all the O_2 molecules are used up in the reaction before all the H_2 molecules can react and the combustion results in some H_2 molecules left over.

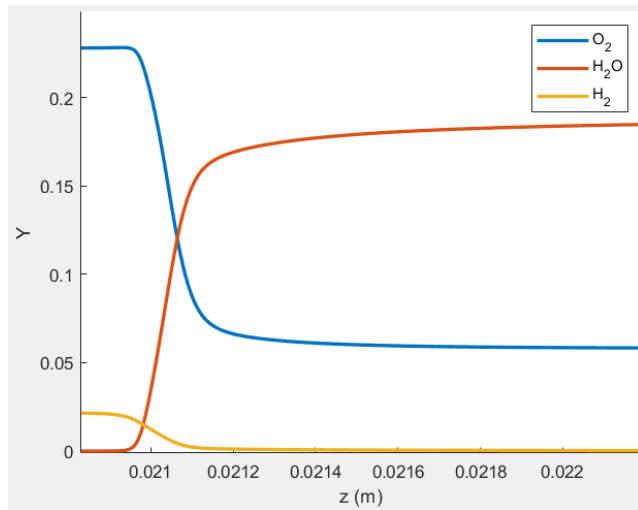


Figure 8 - Mass Fraction of different species for $\Phi = 0.75, P=2\text{atm}$

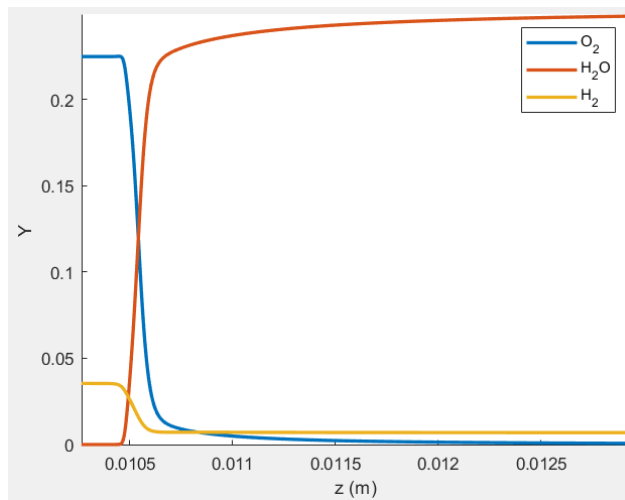


Figure 9 - Mass Fraction of different species for $\Phi = 1.25, P=2\text{atm}$

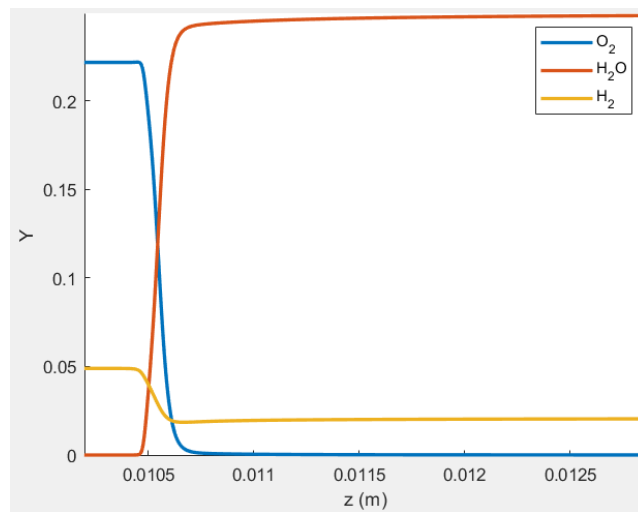


Figure 10 - Mass Fraction of different species for $\Phi = 1.75$, $P=2\text{atm}$

Figure 8, Figure 9 and Figure 10 show the mass fraction of O_2 , H_2O and H_2 at 2 times the atmospheric pressure. The trend for the different mass fractions relative to the equivalence ratio is the same as for the 0.5 atmospheric pressure. The biggest difference is the reaction zone. For the higher initial pressure, the reaction zone is closer in the spatial coordinate. This indicates that the reaction reaches the optimal conditions for combustion faster.

3.4 Heat Release Rate

Measuring Heat Release Rate (HRR) is important to determine the power output of a flame. It is measured in Watt $\left[\frac{J}{s}\right]$. Here the HRR is compared to different equivalence ratios.

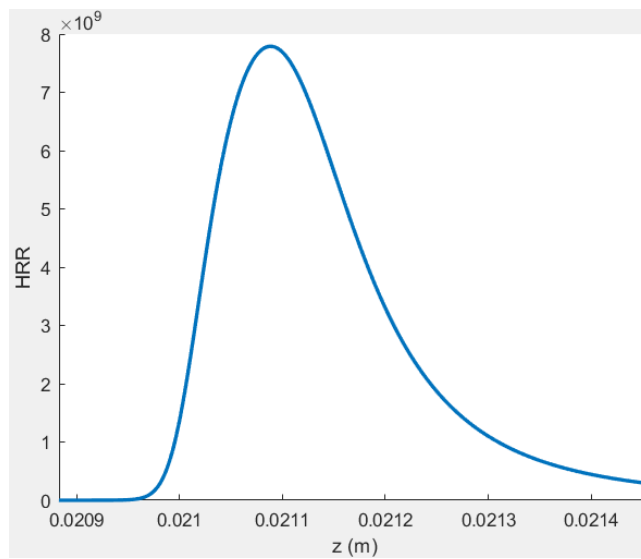


Figure 11 - Heat Release Rate for Phi=0.5, P=2atm

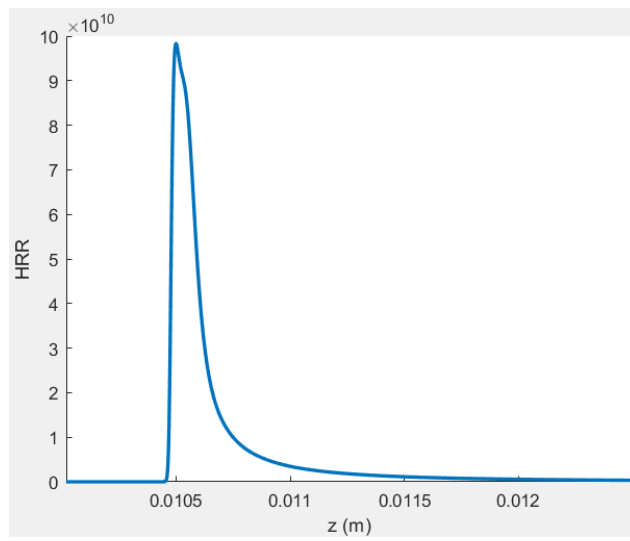


Figure 12 - Heat Release Rate for Phi=1.0, P=2atm

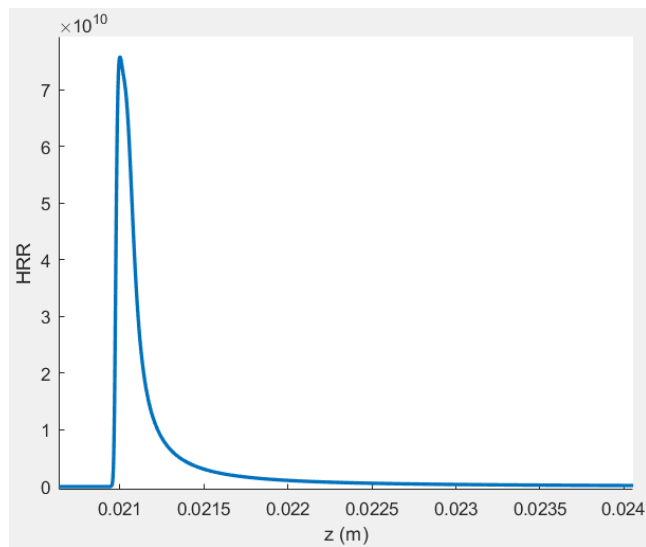


Figure 13 - Heat Release Rate for Phi=1.5, P=2atm

The Figure 11Figure 12Figure 13 and Figure 14 show the highest HRR for Equivalence ratio $\phi = 1.5$. This indicate that the power output of a reaction is related to the Laminar Flame Velocity S_L^0 .

3.5 Other Results

The software Cantera gives a lot of useful numerical results that can be used to study different combustion reactions.

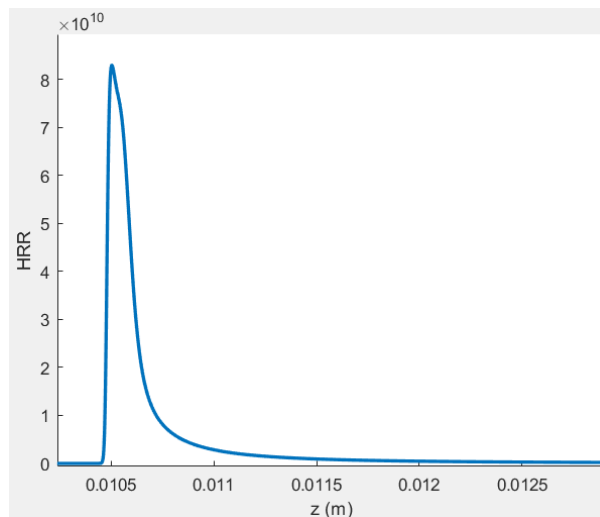


Figure 14 - Heat Release Rate for Phi=2.0, P=2atm

3.5.1 Thermal Conductivity

Thermal conductivity (k) $\left[\frac{W}{mK} \right]$ is the ability to transfer heat. Using the Cantera software this can be calculated for different equivalence ratios, pressures, and temperatures.

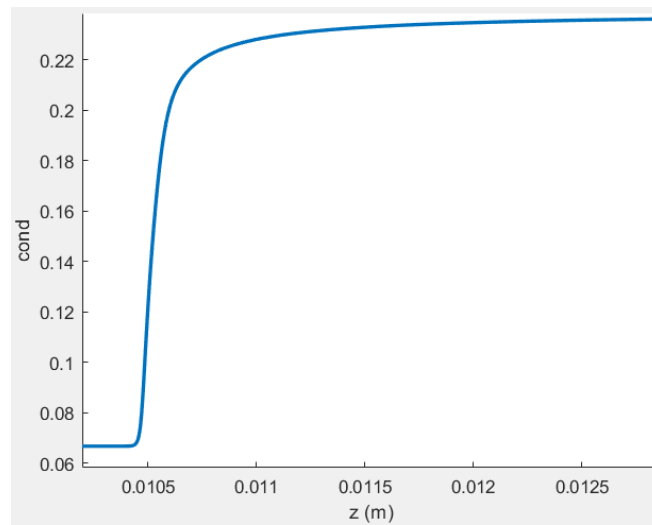


Figure 15 - Thermal Conductivity for hydrogen/air
laminar flame for $\Phi=1.75$ and $P=2\text{atm}$

These computations can be used to present how k is affected by different initial values for the reaction.

3.5.2 Specific Heat Capacity at Constant Pressure and Volume

Heat capacity is the amount of energy that must be added to one unit of a substance in order to increase the temperature by one unit $\left[\frac{J}{kgK}\right]$.

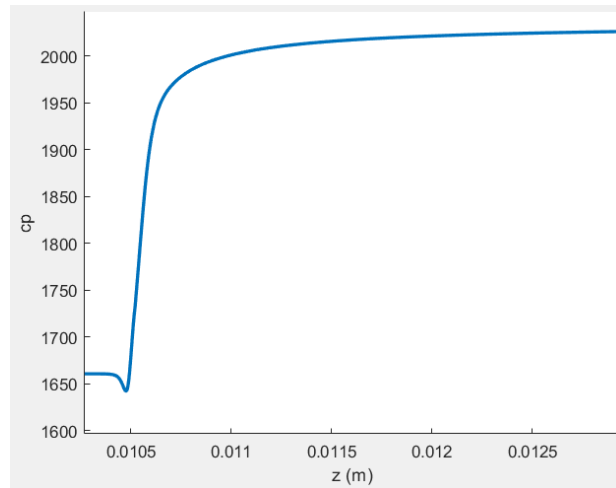


Figure 16 - Specific heat capacity at constant pressure for Hydrogen/air mixture for $\Phi=1.75$, $P=2\text{atm}$

Figure 16 shows the specific heat capacity at constant pressure for hydrogen/air mixture at $\phi = 1.75$ and $P = 2 \text{ atm}$.

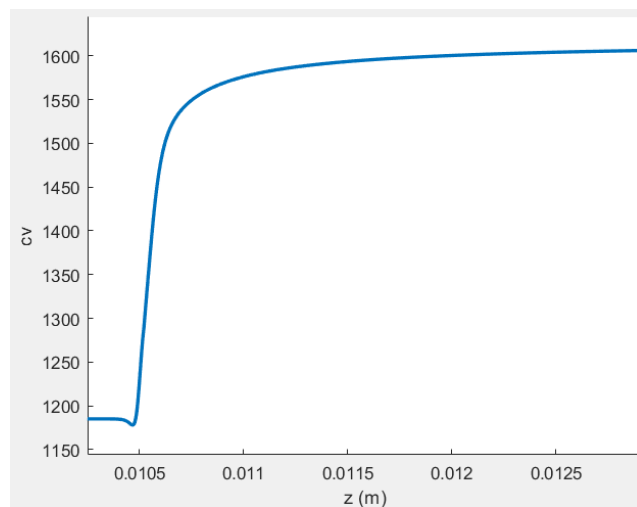


Figure 17 - Specific heat capacity at constant volume for Hydrogen/air mixture for $\Phi=1.75$, $P=2\text{atm}$

Figure 17 shows the specific heat capacity at constant volume for hydrogen/air mixture at $\phi = 1.75$ and $P = 2 \text{ atm}$. The heat capacity is significantly higher for constant pressure where the gas is allowed to expand,

than that for constant volume where the substance is heated in a closed vessel that prevents expansion. Which is mostly the case for most substances, especially gasses.

3.5.3 Mixture Average Diffusion Coefficients

Diffusion Coefficient describes a substances ability to diffuse with respect to another substance $\left[\frac{m^2}{s}\right]$. The higher the diffusivity, the faster the substances diffuse into each other.

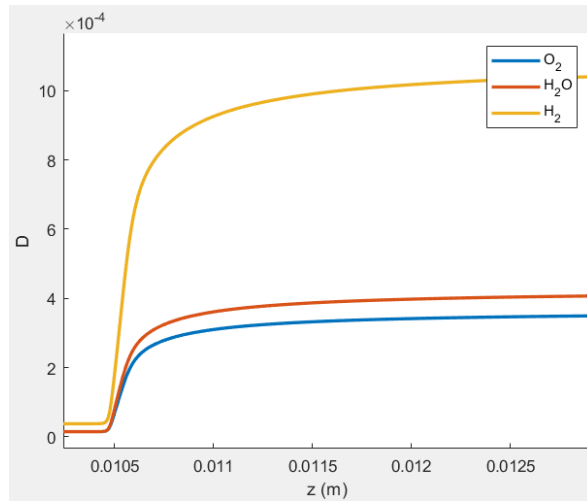


Figure 18 - Mixture Average Diffusion Coefficients for different species for $\Phi=1.75$, $P=2\text{atm}$

3.5.4 Flame Surface Density

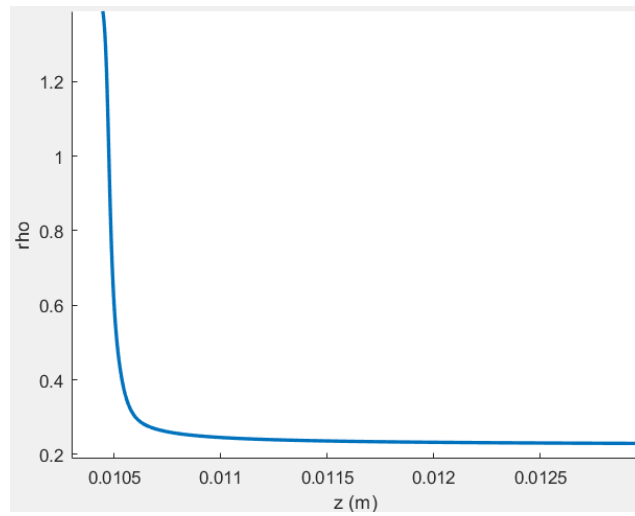


Figure 19 - Flame density for Hydrogen/air laminar flame for $\Phi=1.75$, $P=2\text{atm}$

Flame surface density $\left[\frac{kg}{m^3}\right]$ can be estimated from the transport equations which is what is done by the Cantera software. This parameter can be used to study reaction rate.

3.5.5 Flame Velocity

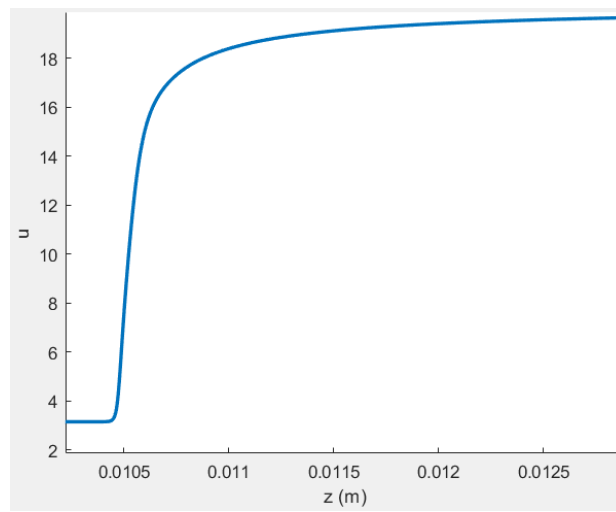


Figure 20 - Flame velocity for Hydrogen/air mixture
for $\Phi=1.75$, $P=2\text{atm}$

Flame velocity $\left[\frac{m}{s}\right]$ is the rate at which the flame front expands in a combustion reaction.

3.5.6 Mole Fraction of Species

Just like the mass fraction, the mole fraction of species can be used to investigate the combustion reaction.

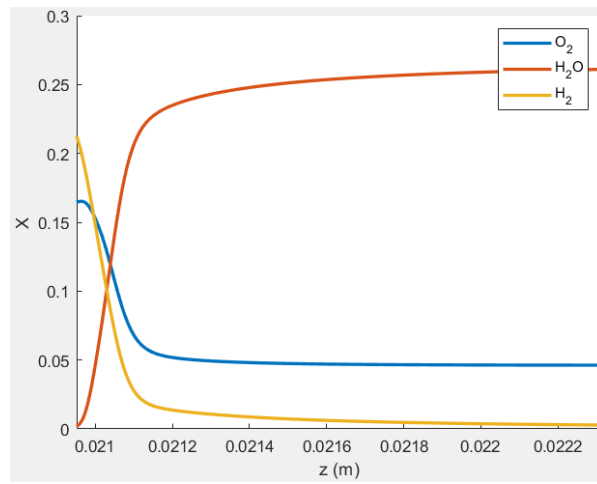


Figure 21 - Mole Fraction of different species for $\Phi = 0.75, P=2\text{atm}$

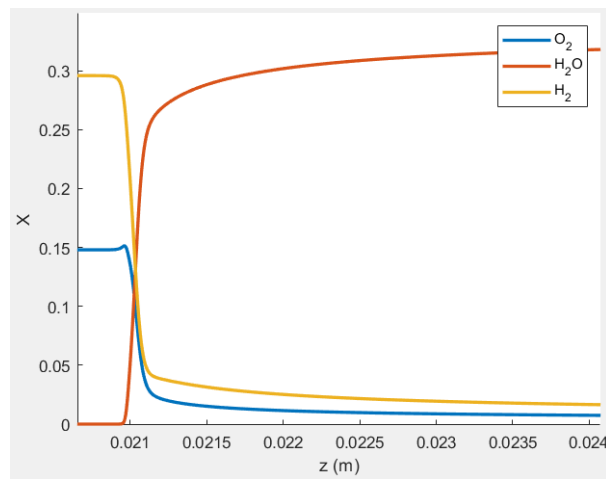


Figure 22 - Mole Fraction of different species for $\Phi = 1.00, P=2\text{atm}$

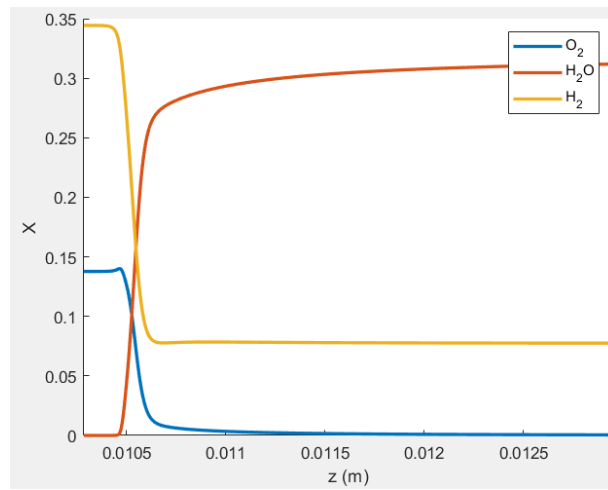


Figure 23 - Mole Fraction of different species for $\Phi = 1.25$, $P=2\text{atm}$

The Figure 21, Figure 22 and Figure 23 show the mole fraction of O_2 , H_2O and H_2 . The plots show that almost all the reactants are used at the stoichiometric ratio.

4. Summary and Conclusion

The aim of this study was to investigate and calculate some values for laminar hydrogen flames. The results discovered show some of the important properties of hydrogen combustion needed to make the switch from carbon-based fuels to carbon neutral or even carbon free hydrogen fuel. This study shows a method that can be used to help understand the combustion physics and behaviour, which is an important field where lots of experimental and numerical studies are needed. The chemical kinetics and the Cantera software is one of many available methods of performing numerical calculations on combustion processes. All the difficult calculations were made automatically by the software, but all the results needed to be interpreted in a meaningful way.

The Laminar Flame Velocity S_L^0 has been found to be highest for equivalence ratio $\phi = 1.5 - 1.75$. It peaks at around 3 m/s and is the highest for 2 times the atmospheric pressure [*atm*]. Low pressure decreases the top S_L^0 , but increasing the pressure above 2 atm does not increase it either. Calculations performed in this study indicate that the S_L^0 is highest for 2 times the atmospheric pressure and reaches 3.15 m/s . This is much higher than that of for example natural gas which is 0.41 m/s for equivalence ratio $\phi = 1.1$ (1). The higher S_L^0 means that the hydrogen can burn at a lean mixture with less fuel and more air and still burn at a similar rate as the natural gas, using less fuel. At equivalence ratio $\phi = 0.5$ the laminar flame velocity is still higher than 0.41 m/s for natural gas and is 0.43 m/s at 2 atm . The heat release rate (HRR) at these conditions is still almost 8% of that of the maximum HRR for hydrogen-air mixture found in this study.

This study shows that this numerical method gives reliable results and can be an easier and cheaper way of studying combustion, alongside the physical research. The results from the computation can be used for further generation

of combustion models and development of renewable fuels. It is shown that the computations are easy to perform, and the different parameters can easily be change in order to investigate different models.

Finally, this study shows that using hydrogen as an alternative to fossil fuels is a viable solution and should be one of the main fields of research and development on the way to carbon neutral and even carbon free future.

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