Faculty of Power and Aeronautical Engineering
Institute of Heat Engineering

Computational Methods in Combustion

IMPACT OF PRESSURE AND FUEL COMPOSITION ON IGNITION TIMING AND FLAME TEMPERATURE

Author:
Mateusz Kucharski

Supervisor:
dr inż. Mateusz Żbikowski

June, 2023

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1 Introduction

The project explores the relationship between pressure, fuel composition, and the auto-ignition characteristics of different fuels. Understanding the ignition timing and flame temperature of fuels is crucial in various fields, including combustion research, engine design, and safety considerations. The field of investigation focus on three different fuels: hydrogen (H2), methane (CH4), and ethane (C2H6). These fuels are widely used in various applications and understanding their ignition properties under different conditions is essential for optimizing combustion processes. The main focus of the project is to analyze the effect of pressure and fuel composition on the auto-ignition time and flame temperature of the selected fuels. Auto-ignition time refers to the time required for a fuel-air mixture to spontaneously ignite without the need for an external ignition source. Flame temperature, on the other hand, represents the maximum temperature reached during the combustion process. To conduct the analysis, a computational approach utilizing the Cantera software library. To simulate the combustion program utilizes a constant-temperature reactor and a constant-pressure reactor to simulate the process under controlled conditions. By varying the pressure and fuel composition, the project aims to observe the impact on the ignition timing and flame temperature for each fuel. The results of the analysis are presented graphically, showing the variation in flame temperature over time for different pressure levels and fuel compositions.

2 Computional methods

The combustion simulations were performed using the Cantera library, which is a powerful tool for solving chemical kinetics problems. Cantera provides a comprehensive set of functions and classes for modeling reactive systems. In this code, the Ideal Gas Reactor models from Cantera were utilized to simulate the combustion processes. Two types of reactors were employed: constant temperature and constant pressure reactors.

2.1 Initial conditions

- The simulations were initialized with an initial temperature (T) and pressure (P) for each case analyzed.
- The initial temperature was set to 1000K.
- The initial pressure was varied in the range of 5 to 15 atm for hydrogen and methane, and 5 to 10 atm for ethane.

2.2 Cases analyzed

1. **Hydrogen:**
    - Three different molar compositions of hydrogen (H2) were considered: 10%, 30%, and 70% by volume.
    - Simulations were performed at different pressures (5 atm, 10 atm, and 15 atm) using a constant temperature reactor.
2. **Methane:**
    - Three different molar compositions of methane (CH4) were investigated: 10%, 30%, and 70%.
    - Simulations were carried out at pressures of 5 atm, 10 atm, and 15 atm using a constant temperature reactor.
3. **Ethane:**
    - Three different molar compositions of ethane (C2H6) were studied: 10%, 30%, and 70%.
    - Simulations were conducted at pressures of 5 atm, 10 atm, and 15 atm using a constant temperature reactor.

3 Results

The simulations provided valuable insights into the auto-ignition behavior of the different fuel-air mixtures at varying pressures. The following observations were made:

3.1 Hydrogen

- At a constant temperature of 1000K, an increase in the hydrogen concentration resulted in longer auto-ignition times. The 10% hydrogen composition exhibited the shortest ignition delay, followed by 30% hydrogen and 70% hydrogen.
- Increasing the pressure from 5 atm to 15 atm led to a decrease in the auto-ignition time for all hydrogen compositions. Higher pressures resulted in shorter ignition delays, indicating the promoting effect of pressure on hydrogen auto-ignition.

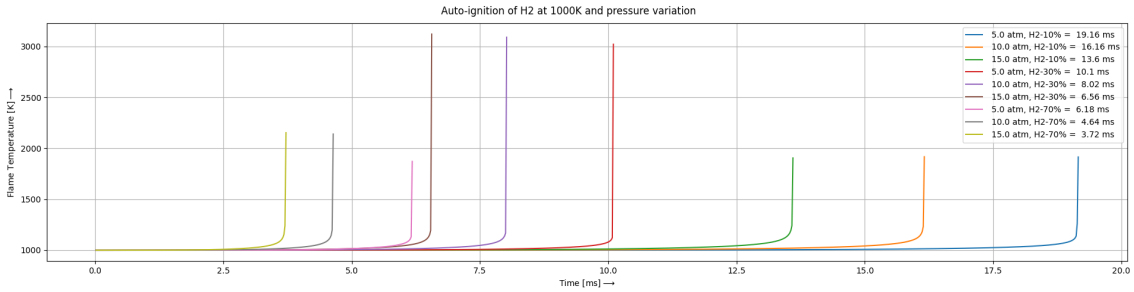

Figure 1: Influence of preassure and fuel concentration

3.2 Methane

- Similar to hydrogen, an increase in methane concentration led to longer auto-ignition times. The 10% methane composition showed the shortest ignition delay, followed by 30% methane and 70% methane.
- Increasing the pressure from 5 atm to 15 atm also resulted in shorter auto-ignition times for methane mixtures. Higher pressures exhibited a promoting effect on the ignition process.

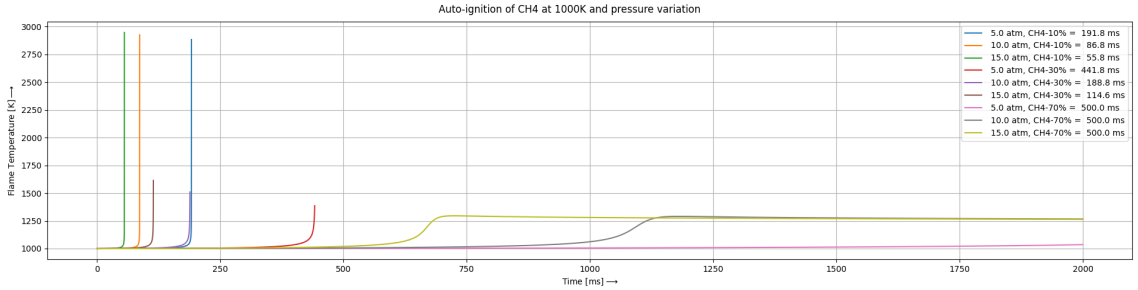

Figure 2: Influence of preassure and fuel concentration

3.3 Ethane

- Ethane exhibited a similar trend to hydrogen and methane, with higher concentrations leading to longer auto-ignition times. The 10% ethane composition resulted in the shortest ignition delay, followed by 30% ethane and 70% ethane.
- Pressure variations had a similar effect on the ignition delay in ethane mixtures. Increasing the pressure from 5 atm to 15 atm resulted in a decrease in the auto-ignition time, indicating the promoting influence of higher pressures.

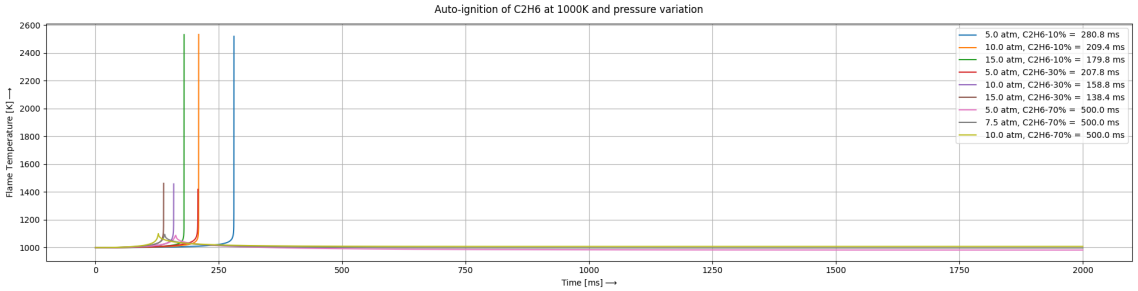

Figure 3: Influence of preassure and fuel concentration

Overall, the simulations revealed that an increase in fuel concentration tended to prolong the auto-ignition time, while an increase in pressure resulted in shorter ignition delays for hydrogen, methane, and ethane mixtures. These findings highlight the complex interactions between fuel composition and pressure in determining the ignition characteristics of these fuels in practical combustion systems.

4 Conclusions

In this study, the auto-ignition behavior of hydrogen, methane, and ethane mixtures was investigated using computational simulations. The results provide insights into the influence of fuel composition and pressure on the ignition characteristics of these fuels.

The analysis revealed that hydrogen exhibited the shortest ignition time among the tested fuels. This can be attributed to the unique properties of hydrogen, such as its high reactivity and wide flammability limits. The rapid kinetics and high energy release of hydrogen contribute to its fast ignition, even at lower concentrations and pressures.

On the other hand, methane and ethane demonstrated longer ignition times compared to hydrogen. This can be attributed to their lower reactivity and slower combustion kinetics. As the concentration of methane or ethane increased in the fuel-air mixture, the ignition time tended to increase, indicating the need for more time for the reactants to reach the critical conditions for self-ignition.

Regarding pressure, an increase in pressure generally resulted in shorter ignition delays for all tested fuels. Higher pressures provide favorable conditions for enhanced fuel-air mixing, increased reactant collision frequency, and elevated reaction rates. These factors contribute to the promotion of the auto-ignition process, leading to shorter ignition delays.