Faculty of Power and Aeronautical Engineering
Institute of Heat Engineering

Computational Methods in Combustion

Autoigniton of Stoichiometric Mixtures of Ethane and Propane with Air and Oxygen for Varying Initial Conditions

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1 Introduction

The phenomenon of a mixture of gases burning spontaneously without an external source of ignition is called autoignition. Nevertheless, there is a time that passes between the initiation of a combustion process and the moment the mixture reaches the critical temperature for the combustion to actually occur - the ignition delay. Ignition delay describes the period before the mixture reaches parameters at which self-sustained combustion can propagate.

Autoignition time of ethane and propane is a parameter that is crucial in the design and optimization of combustion processes in numerous industrial and environmental applications. These hydrocarbons are widely used throughout fields such as power and aerospace engineering, hence investigating the conditions at which the reactants work can provide valuable insights into the processes that are so common in the modern engineering world.

The aim of the project was to simulate autoignition of ethane and propane under different initial conditions and draw conclusions from their influence on ignition delay. The following four mixtures were subjected to simulation: ethane with air, ethane with oxygen, propane with air, and propane with oxygen.

For all considered cases, the same autoignition condition was applied. All simulations recognized ignition delay as the time needed to achieve a spike in the temperature of more than 400K.

2 Simulation

All simulations described were conducted using Cantera, a software tool for the Python environment.

The chemical kinetic model used to replicate the behavior of ethane and propane was Cantera's built-in GRI Mech 3.0. Depending on the type of simulation, constant temperature vs. constant pressure, different types of Cantera's gas reactors were utilized.

In all cases stiochimoetric combustion was conducted. Reactions of burning specific mixtures are presented below:

$$C_2H_6 + 3.5\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O$$

$$C_2H_6 + 3.5\ O_2 + 13.16\ N_2 \rightarrow 2\ CO_2 + 3\ H_2O + 13.16\ N_2$$

$$C_3H_8 + 5\ O_2 + 18.8\ N_2 \rightarrow 3\ CO_2 + 4\ H_2O + 18.8\ N_2$$

$$C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O$$

2.1 Autoignition with constant temperature and varying pressure

This study investigated how varying pressure affects the autoignition time of ethane and propane at a constant temperature of 1100 K, ranging from 1 to 4 atmospheres. The findings shed light on how pressure influences the ignition properties of considered hydrocarbons.

2.2 Autoignition with constant pressure and varying temperature

The study examined how temperature affects the autoignition time of ethane and propane while maintaining a constant pressure of 3 atmospheres. The temperature range explored was from 1000 K to 1200 K. This analysis reveals the thermal sensitivity of hydrocarbons combustion.

3 Results

3.1 Ethane mixtures with constant temperature

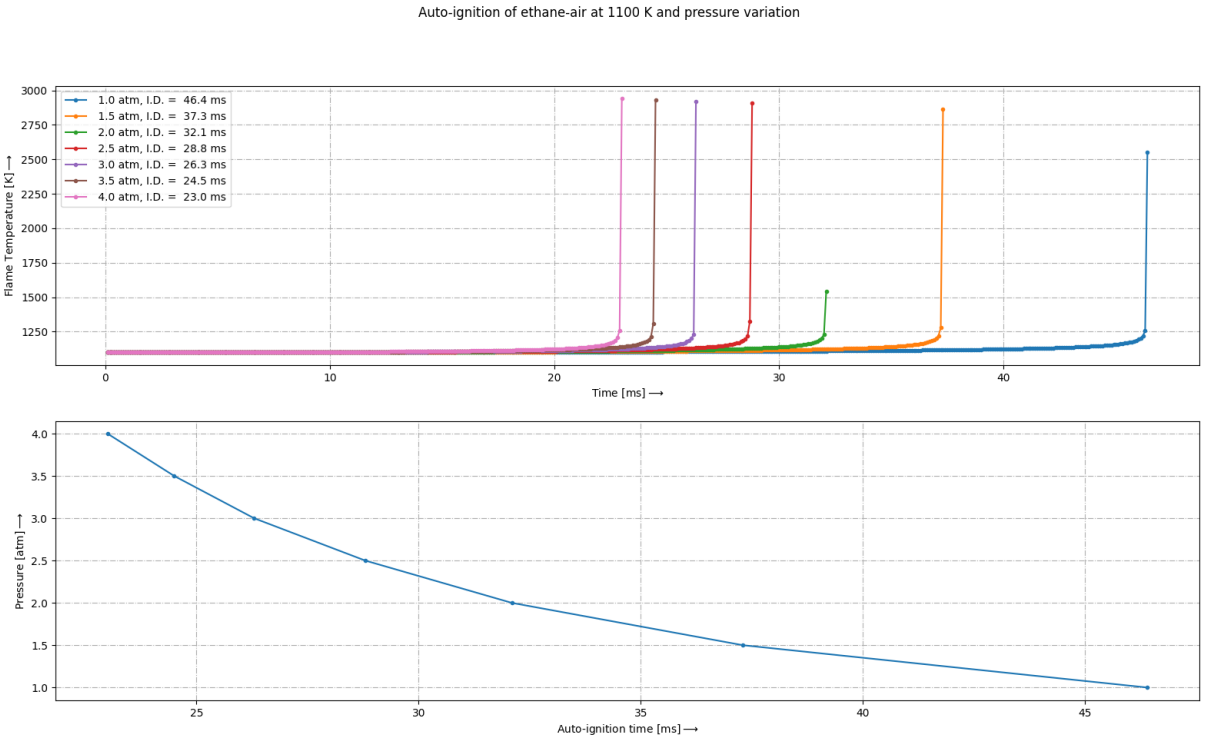

Figure 3.1: Ethane-air at 1100K

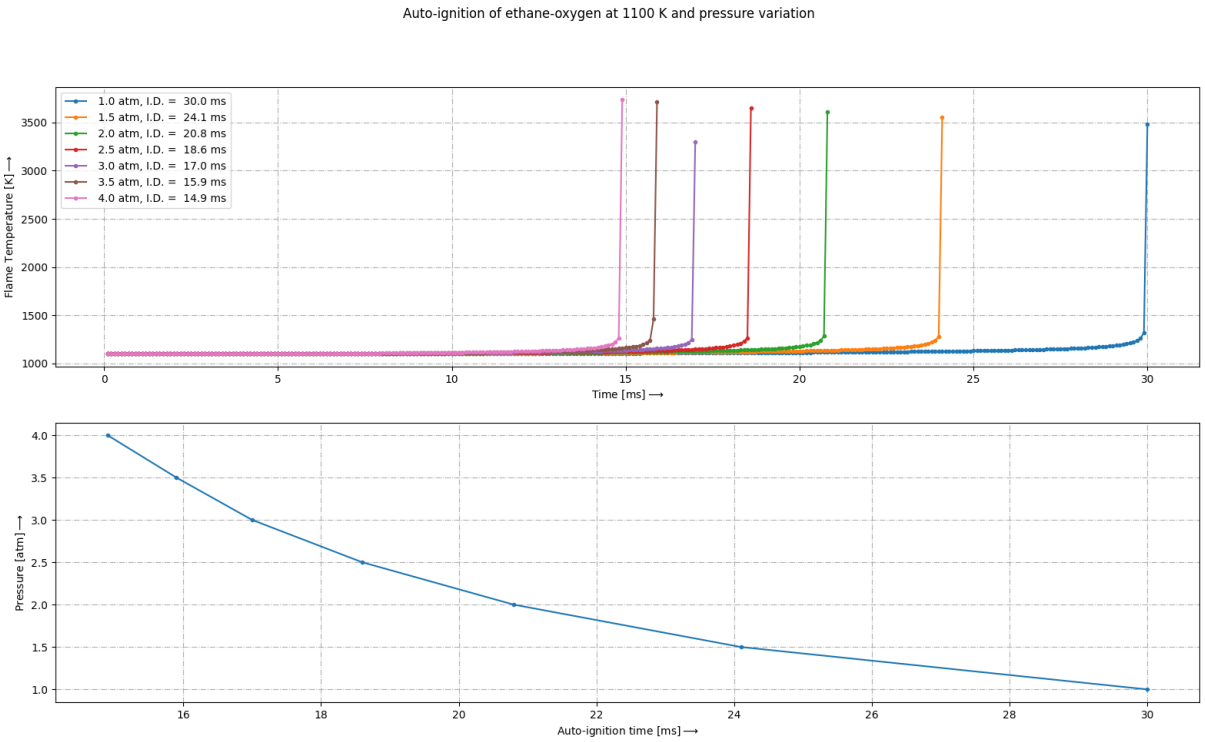

Figure 3.2: Ethane-oxygen at 1100K

3.2 Propane mixtures with constant temperature

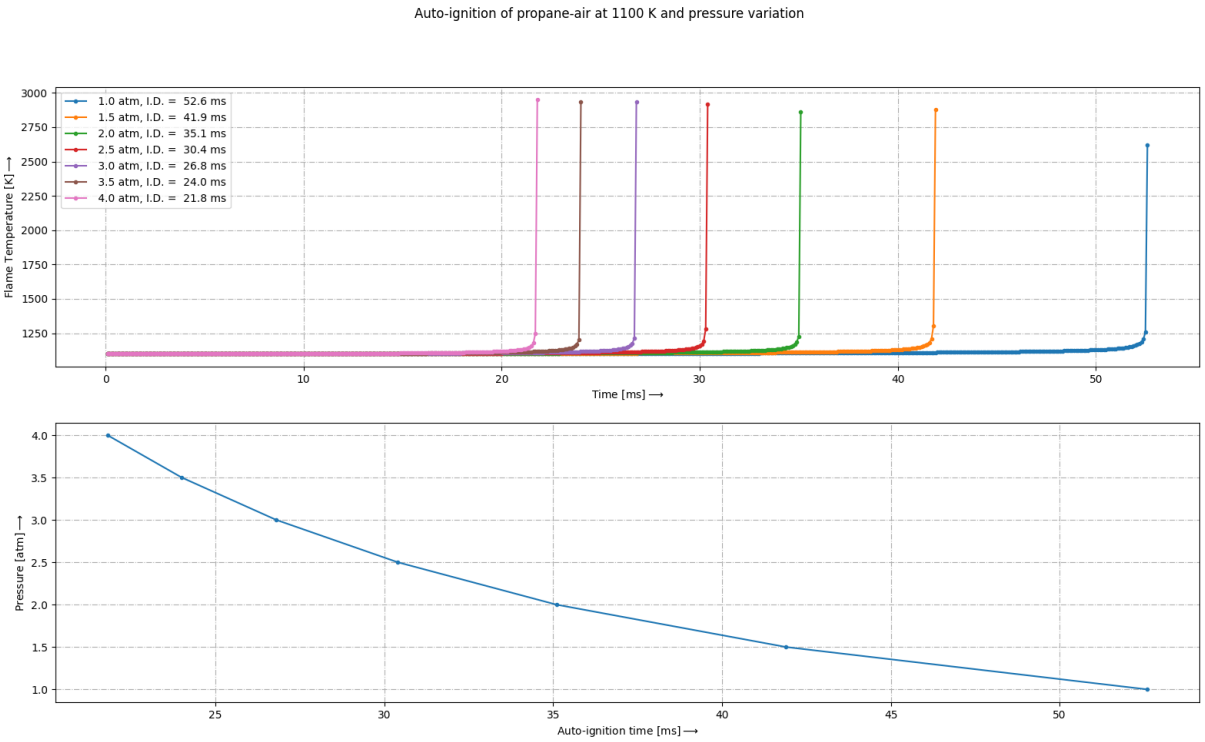

Figure 3.3: Propane-air at 1100K

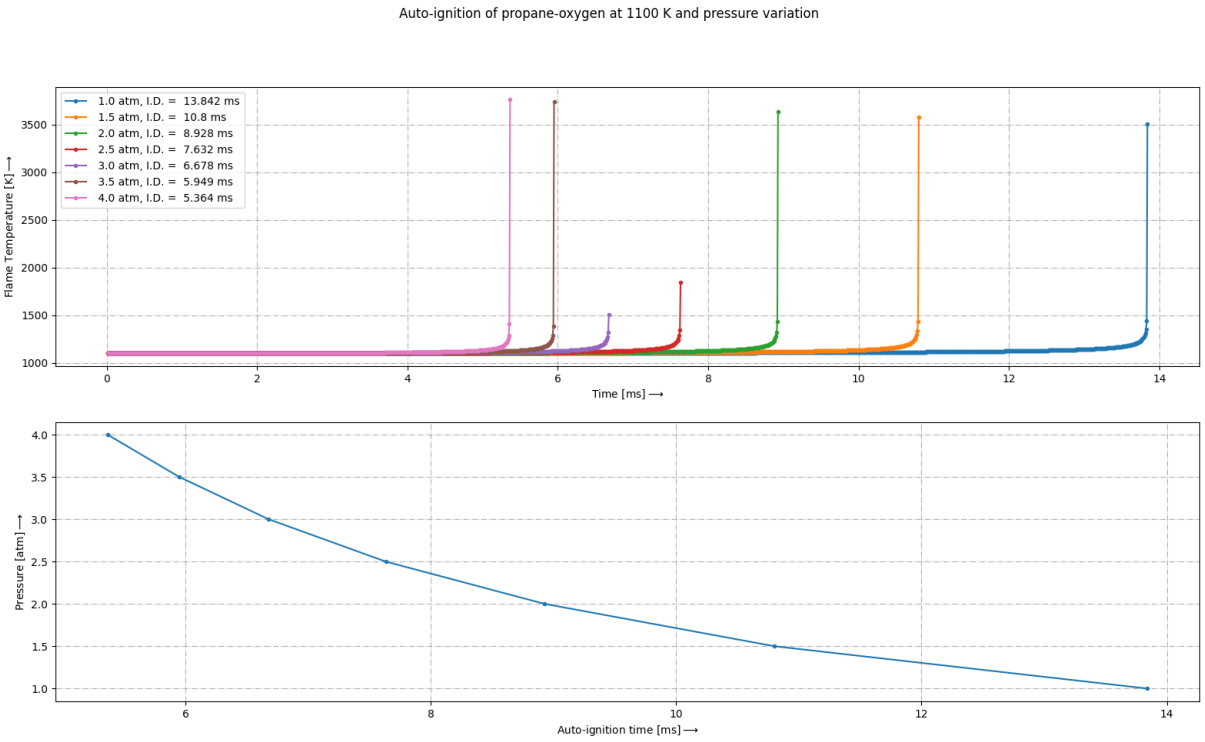

Figure 3.4: Propane-oxygen at 1100K

3.3 Ethane mixtures with constant pressure

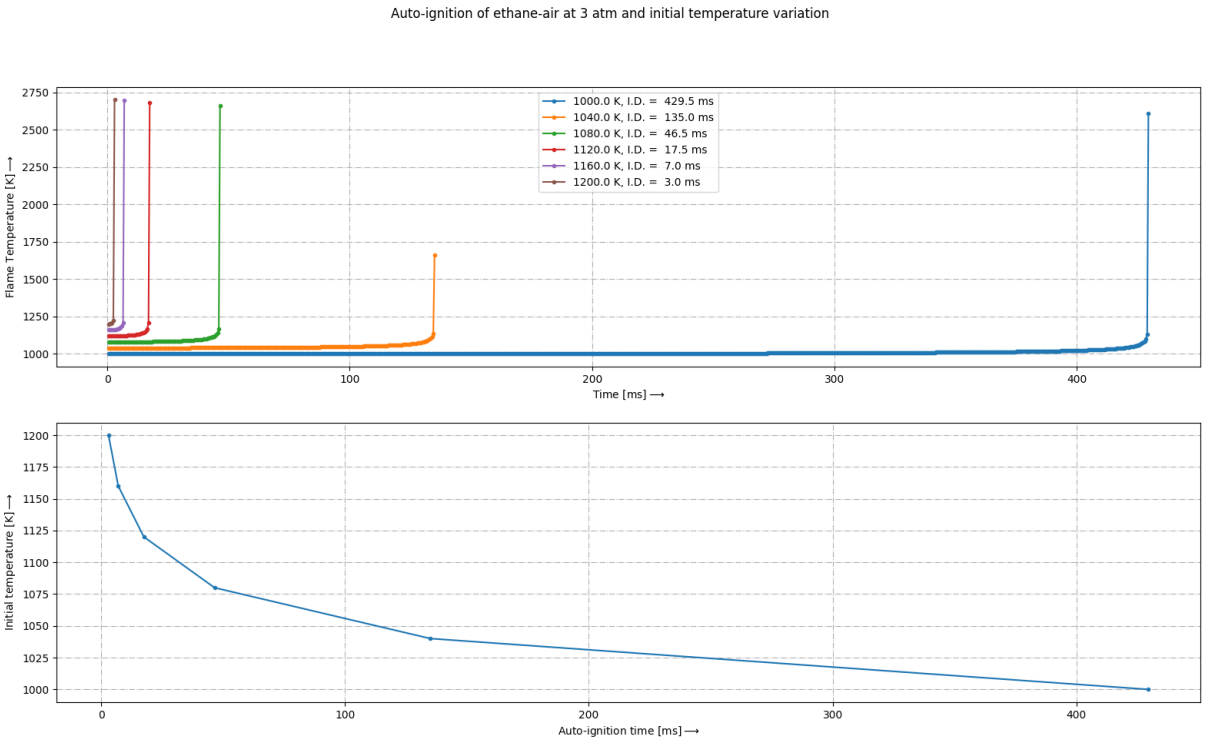

Figure 3.5: Ethane-air at 3 atm

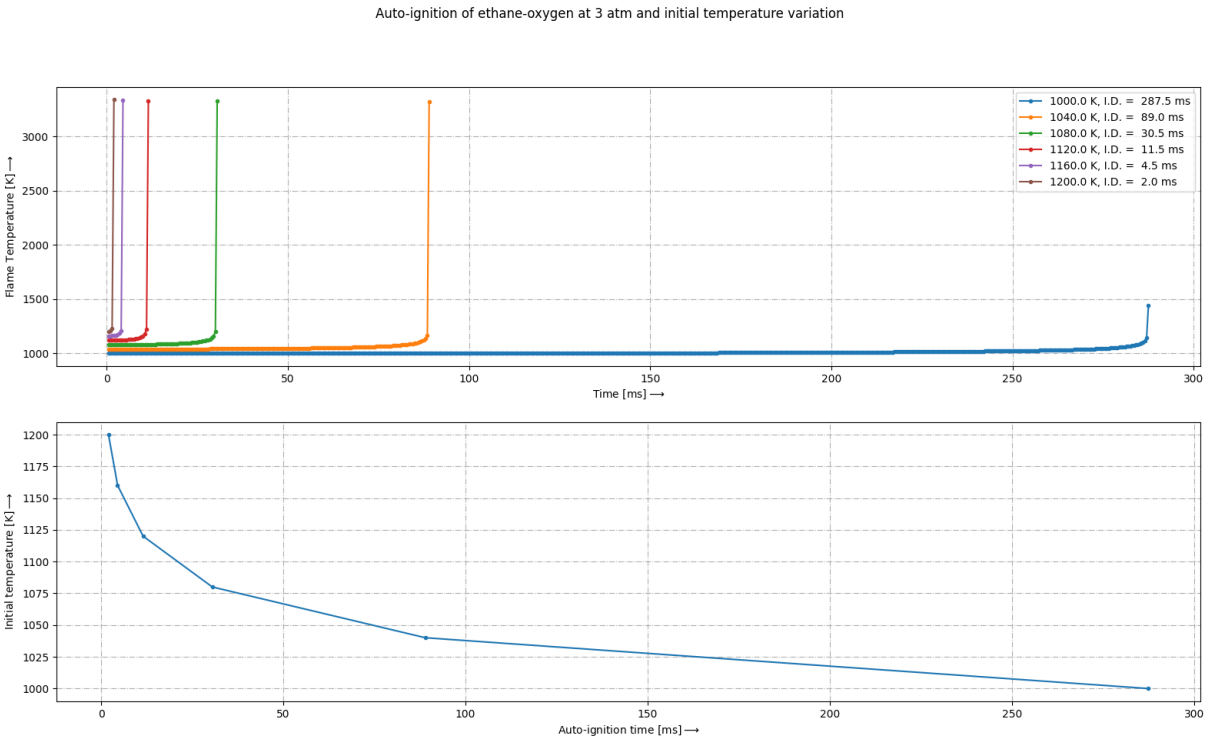

Figure 3.6: Ethane-oxygen at 3 atm

3.4 Propane mixtures with constant pressure

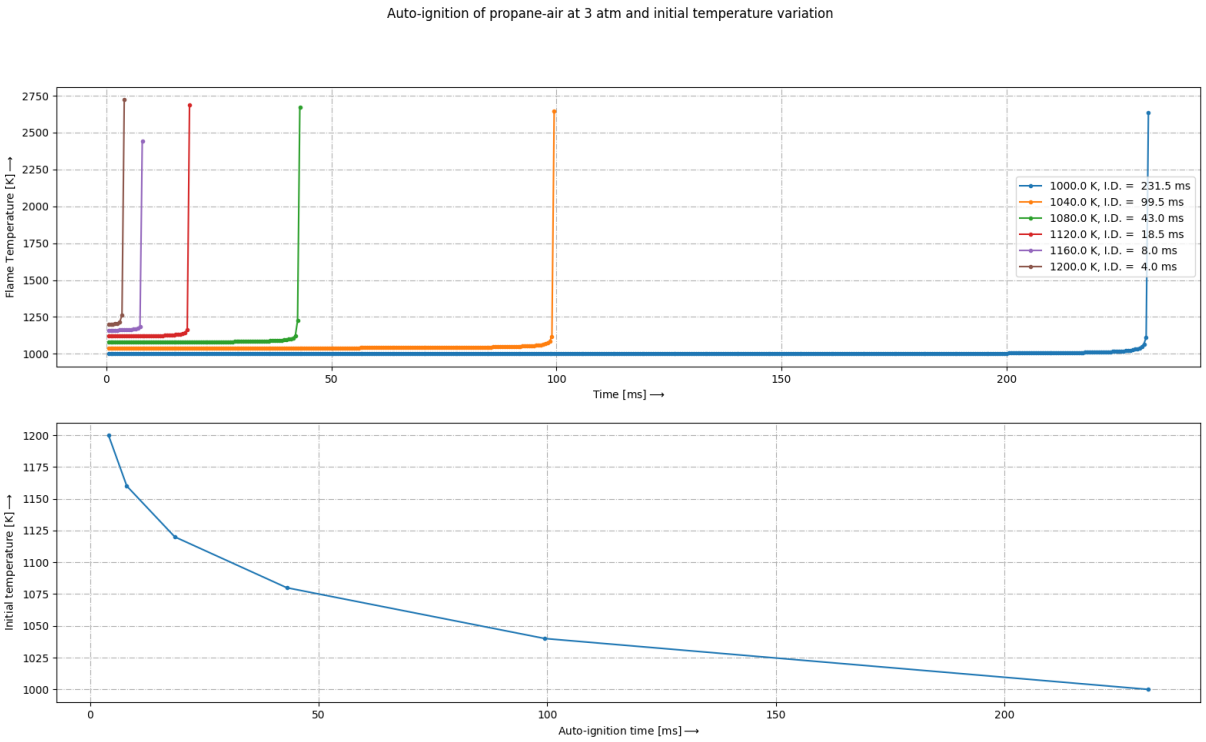

Figure 3.7: Propane-air at 3 atm

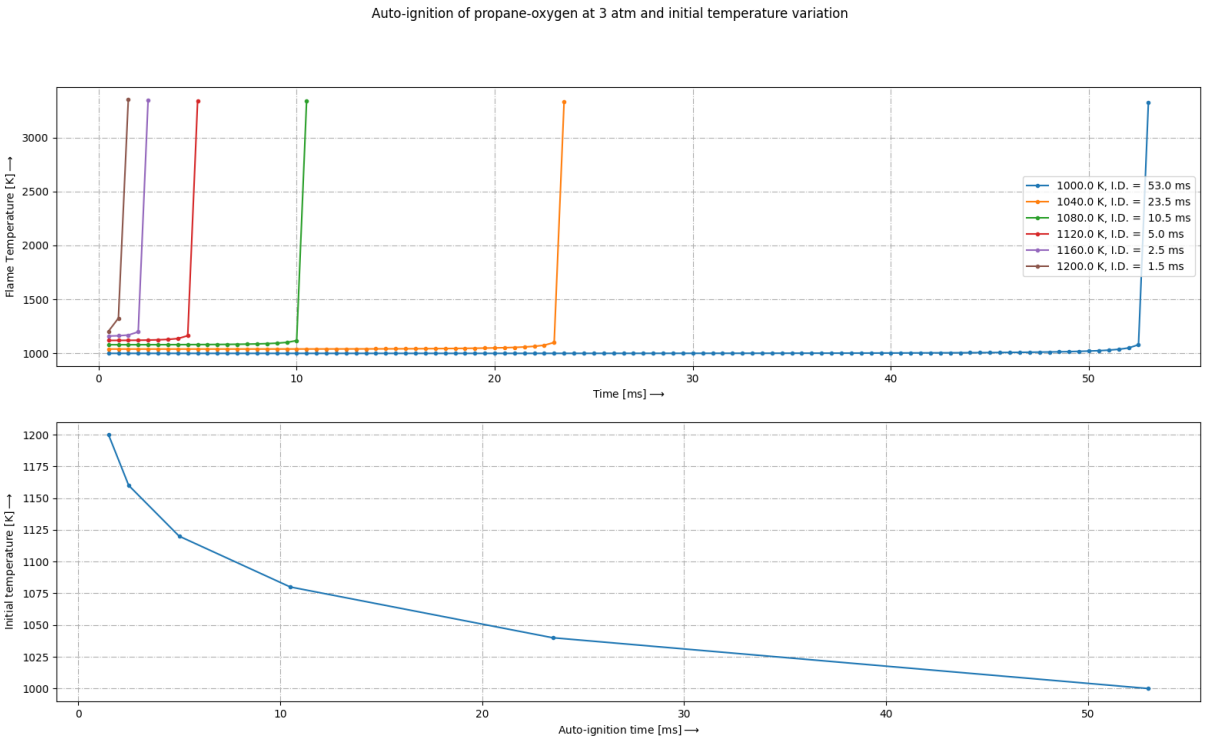

Figure 3.8: Propane-oxygen at 3 atm

4 Conclusions

After the ignition time, the temperature of the mixtures rises rapidly, the process is very quick. Analyzing the composition of mixtures, it can be seen that in the case of mixtures of hydrocarbons with oxygen, the ignition delay time is significantly shorter than in the case of mixtures of the same hydrocarbons with air. For propane mixtures at constant temperature and pressure of 4 atmospheres the difference in ignition delay time is more than 15ms - the ignition delay time for a propane-oxygen mixture is more than 4 times shorter than for a propane-air mixture. The presence of oxygen significantly enhances the auto-ignition process for both ethane and propane compared to air. Oxygen, being a more reactive oxidizer than air, facilitates faster combustion, making it more suitable for applications requiring rapid ignition and high combustion efficiency.

Under constant pressure conditions and the initial temperature above 1150K, the ignition delay time for mixtures of both hydrocarbons is similar. Also for constant pressure conditions, it can be noted that a relatively small increase in temperature (40K) can reduce the ignition delay time by more than three times - the case of ethane-air mixture.

For the assumed initial conditions, the change in temperature has a greater effect on the autoignition delay time. According to the plots, the ignition delay time decreases asymptotically with increasing initial mixture temperature. Nevertheless, increasing initial pressure of the mixture also reduces autoignition delay time.

For both cases of propane-oxygen mixtures under both constant pressure and constant temperature conditions, the ignition delay time is shorter than in the case for ethane-oxygen mixtures. Due to the conditions of constant pressure or constant temperature, a similar conclusion cannot be unequivocally made for hydrocarbon-air mixtures.

5 References

[1] ‘Simulating auto ignition using Cantera’, Kshitiz Sahai
[2] https://github.com/JakubCzerniej/MKWS_project