Faculty of Power and Aeronautical Engineering
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Computational methods in combustion

Influence of temperature and pressure on autoignition delay time

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1. Introduction

Autoignition is a process accomplished when certain gas mixture ignites without any external source of ignition such as spark or flame. This phenomenon occurs after reaching a certain temperature called autoignition temperature. Autoignition temperature is the lowest temperature in which the process can occur. It is being determined for normal atmosphere and the mixture of gases or vapours with oxidizer.
Autoignition delay time is the time that takes for a mixture of fuel and air to self-ignite. This time is dependant on few factors including:

· Temperature
· Pressure
· Substance

Understanding and control of this property allows for improvements in engine performance by optimizing combustion process and reducing emissions as well as developing more efficient fuels.

2. Cases analysed

For the purpose of the project two mixtures were analysed:

- Methane with oxygen
- Hydrogen with oxygen

Stoichiometric reactions were applied:

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$
$$2H_2 + O_2 \longrightarrow 2H_2O$$

Case 1: Influence of temperature on autoignition delay time for: 5 atm of initial pressure, simulation time: 5 s with 0.001 s step time.
Case 2: Influence of pressure on autoignition delay time for: 1000 K of initial temperature, simulation time: 5 s with 0.001 s step time.

3. Computational method

For purpose of the project autoignition delay time was computed as the time of reaching temperature 400 K greater than the initial temperature by the mixture. Simulation used Cantera software via Python module utilizing chemical kinetic model defined in GRI Mech 3.0.

4. Results

Below are graphs presenting effects of initial temperature and pressure on autoignition delay time for methane-oxygen and hydrogen-oxygen mixtures:

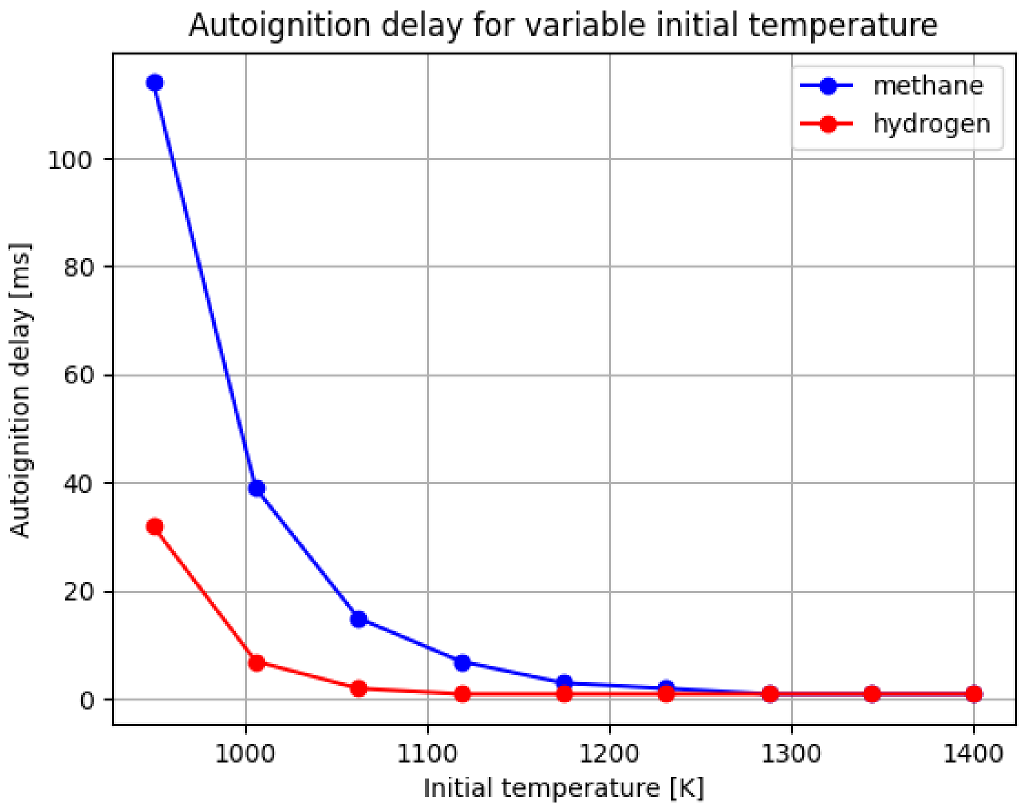

Figure 4.1. Autoignition delay for variable initial temperature

	Time [ms]	
Temperature [K]	Methane	Hydrogen
950	114	32
1006.25	39	7
1062.5	15	2
1118.75	7	1
1175	3	1
1231.25	2	1
1287.5	1	1
1343.75	1	1
1400	1	1

Table 4.1. Autoignition delay for variable initial temperature

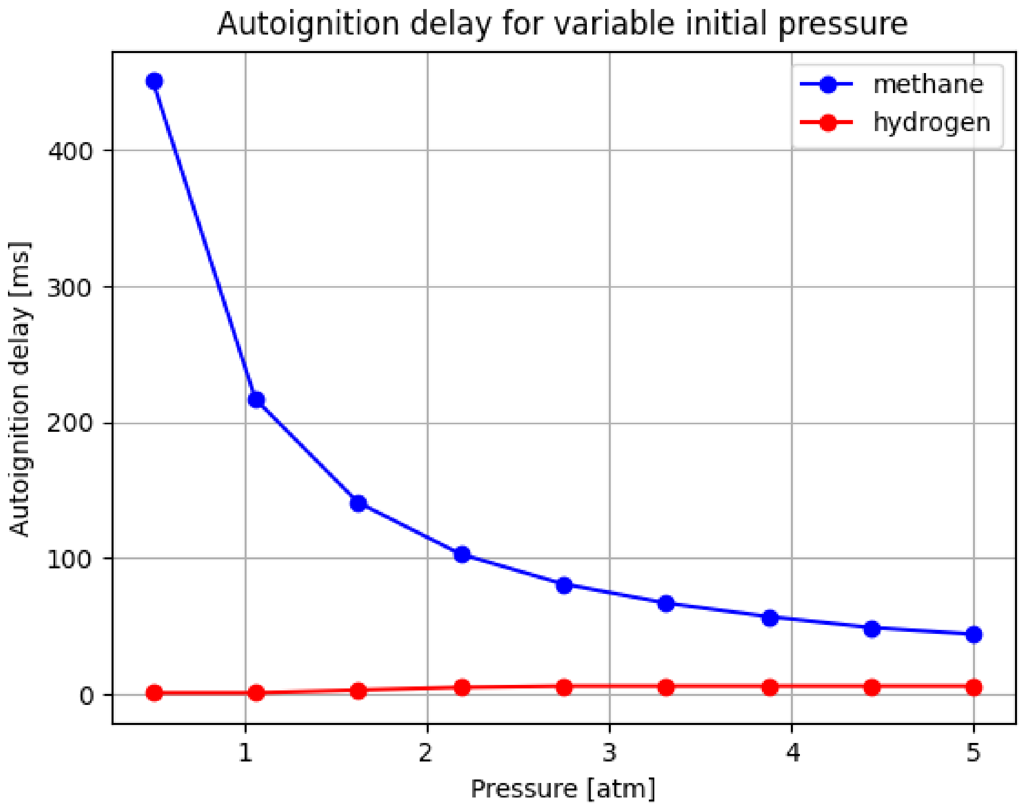

Figure 4.2. Autoignition delay for variable initial pressure

	Time [ms]	
Pressure [atm]	Methane	Hydrogen
0.5	451	1
1.0625	217	1
1.625	141	3
2.1875	103	5
2.75	81	6
3.3125	67	6
3.875	57	6
4.4375	49	6
5	44	6

Table 4.2. Autoignition delay for variable initial pressure

5. Conclusions

- Autoignition delay time decreases as temperature increases for both methane and hydrogen mixtures.
- In case of increasing pressure, autoignition delay time decreases for methane, and increases slightly for hydrogen, however by a negligible amount.
- For methane, the time decreases more drastically with increase in temperature or pressure, generally it's longer than for hydrogen.
- Above 1100 K the autoignition delay time for hydrogen gets so low, that further changes aren't possible to detect with the computational method used. It's also extremely low for the entire range of pressures used in study.
- The decrease in autoiginition delay time is caused by increase in energy of reacting particles, which causes them to vibrate more strongly and in turn react quicker.