Faculty of Power and Aeronautical Engineering
Institute of Heat Engineering

Computational Methods in Combustion

INFLUENCE OF TEMPERATURE AND PRESSURE ON AUTOIGNITION DELAY TIME

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1 Introduction

Autoignition occurs when a mixture of gases or vapors ignites spontaneously with no external ignition source and after reaching a certain temperature, the autoignition temperature. The autoignition temperature is not an intrinsic property of the gases or vapors (Kanury 1975), but is the lowest temperature in a system where the rate of heat evolved from the gases or vapors increases beyond the rate of heat loss to the surroundings, resulting in ignition.
Autoignition delay time refers to the time it takes for a fuel-air mixture to spontaneously ignite without an external ignition source, such as a spark or flame. It depends on several factors, including the fuel composition, temperature, pressure, and the presence of any additives or contaminants.
Autoignition delay time is a critical parameter in the study of combustion kinetics, engine design, and fuel development. Understanding and controlling this characteristic can help improve engine performance, optimize combustion processes, and reduce emissions.

2 Computational method

2.1 Assumptions

For current problem auto ignition delay is calculated as time for achieving temperature 400K higher than initial temperature:

$$t_{ignition.delay} = t_{initial.temp+400K}$$

Calculations was conducted for stoichiometric reacions:

$$CH_4 + 2(O_2 + 3.76N_2) = CO_2 + 2H_2O + 7.52N_2$$

$$C_2H_6 + 3.5(O_2 + 3.76N_2) = 2CO_2 + 3H_2O + 13.16N_2$$

$$C_3H_8 + 5(O_2 + 3.76N_2) = 3CO_2 + 4H_2O + 18.8N_2$$

2.2 Simulation

The simulation was conducted using Cantera, which is a software tool for Python language.
The chemical kinetic model utilized in the study includes GRI Mech 3.0, which is a widely-used reaction mechanism for natural gas combustion. It contains 53 species composed of the elements H, C, O, N, and/or Ar, and 325 reactions, most of which are reversible. GRI-Mech 3.0, like most combustion mechanisms, is designed for use at pressures where the ideal gas law holds.

2.3 Cases analyzed

For the purposes of this project two cases were analyzed:

- Case 1: Influence of temperature (initial pressure = 5atm, simulation time = 10s with step time = 0.002s, mixtures: methane+air, ethane+air, propane+air)
- Case 2: Influence of pressure (initial temperature = 1100K, simulation time = 10s with step time = 0.002s, mixtures: methane+air, ethane+air, propane+air)

3 Results

Results of performed analysis are presented below:

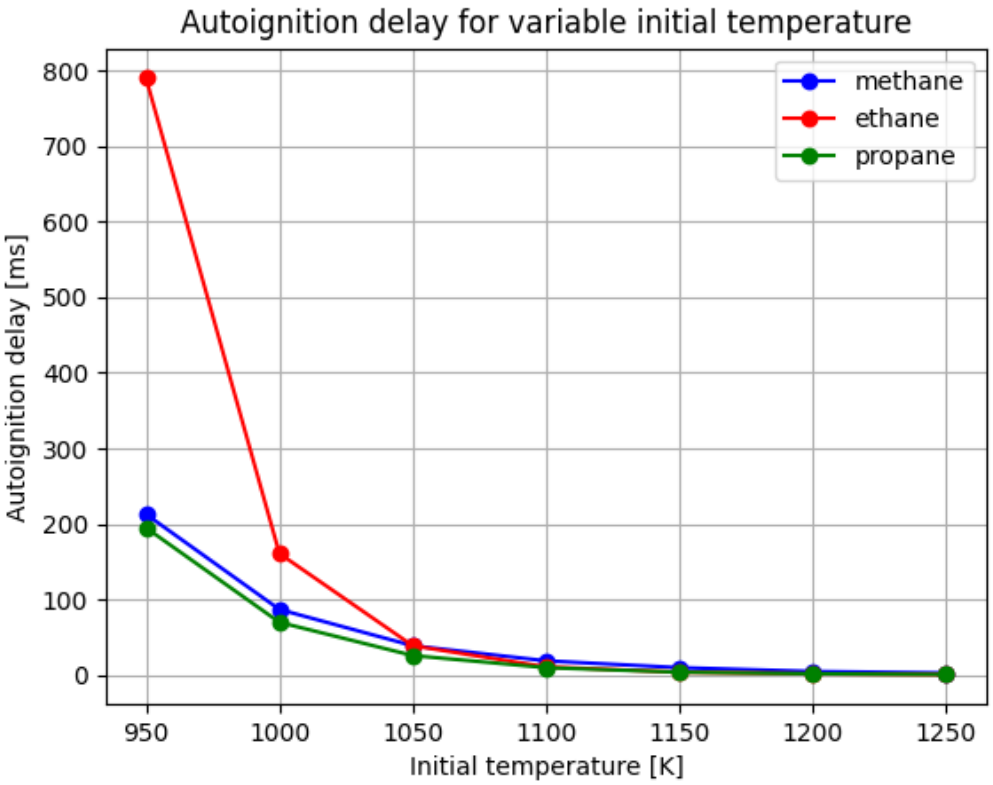

Figure 1: Influence of temperature

	Autoignition delay time [ms]		
Temp [K]	Methane	Ethane	Propane
950	213	790	195
1000	87	161	70
1050	39	39	26
1100	19	11	10
1150	10	4	4
1200	5	2	2
1250	3	1	1

Table 1: Influence of temperature

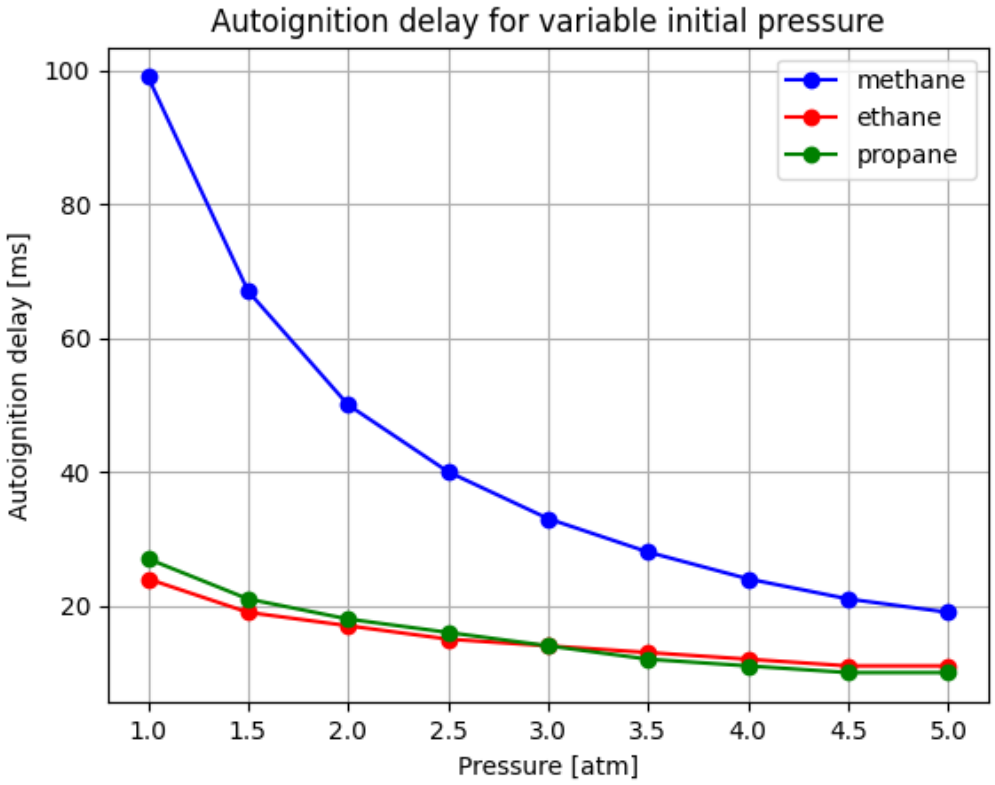

Figure 2: Influence of pressure

	Autoignition delay time [ms]		
Pressure [atm]	Methane	Ethane	Propane
1	99	24	27
1.5	67	19	21
2	50	17	18
2.5	40	15	16
3	33	14	14
3.5	28	13	12
4	24	12	11
4.5	21	11	10
5	19	11	10

Table 2: Influence of pressure

4 Conclusions

- As the temperature increases, the mobility of molecules increases, the lightness decreases (increase in the speed of mixing the fuel and oxidant), and the activation energy decreases - the ignition delay time is shortened
- As the pressure increases, the speed of the chemical reaction increases, and thus the ignition delay time is shortened
- Among the analyzed mixtures, in the analyzed range, temperature has the greatest influence on ethane
- Among the analyzed mixtures, in the analyzed range, pressure has the greatest influence on methane

5 References

- "Safety Design for Space Systems", William D. Manha
- "Analysis of auto ignition temperature and ignition delay using Cantera and Python", Smitesh Badnapurkar
- cantera.org, access on day: 07.06.2023