Faculty of Power and Aeronautical Engineering
Institute of Heat Engineering

Computational Methods in Combustion

AUTOIGNITION OF METHANE FOR VARYING INITIAL CONDITIONS

Influence of molar fuel composition on ignition delay

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1 Objective

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 methane is a parameter that is crucial in the design and optimization of combustion processes in numerous industrial and environmental applications. Methane is 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 methane under different initial conditions and draw conclusions from their influence on ignition delay. Moreover, the molar composition of the 'fuel' was studied in order to expand the number of possible outcomes and further explore the subject. Three cases were examined to exhaustively evaluate the influence of pressure and temperature, as well as the molar composition.

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.

$$t_{\text{ignition time}} = t_{\text{initial temperature+400K}}$$

2 Simulation

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

The chemical kinetic model used to imitate methane's behaviour 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 introduced.

2.1 Autoignition with constant temperature and varying pressure

This case examined the effect of pressure on methane autoignition time while maintaining a constant temperature of 1250 K. Pressure was varied from 1 to 5 atmospheres. The results provide insights into the impact of pressure on methane ignition characteristics.

Combustion of stoichiometric methane mixture in air:

$$CH_4 + 2O_2 + 7.52N_2 \rightarrow CO_2 + 2H_2O + 7.52N_2$$

2.2 Autoignition with constant pressure and varying temperature

Here, the influence of temperature on methane autoignition time was investigated, while keeping the pressure constant at 5 atmospheres. The temperature varied from 950 K to 1450 K. This analysis reveals the thermal sensitivity of methane combustion. Again, a stoichiometric combustion was carried out.

2.3 Autoignition with constant temperature and varying molecular concentration and pressure

In the last case considered, the autoignition time of methane was investigated under a constant temperature of 1250 K while varying the pressure from 1 to 5 atmospheres, hence for the same initial conditions as in the first case. However this time, the molar composition of fuel varied from 0.1 to 0.8 moles of methane for one mole of oxygen. This case aims to examine the influence of pressure and methane concentration on the autoignition characteristics. By analyzing the results, insights can be gained into the ignition behavior of methane under different pressure levels and varying amounts of methane present in the reactant mixture.

3 Results

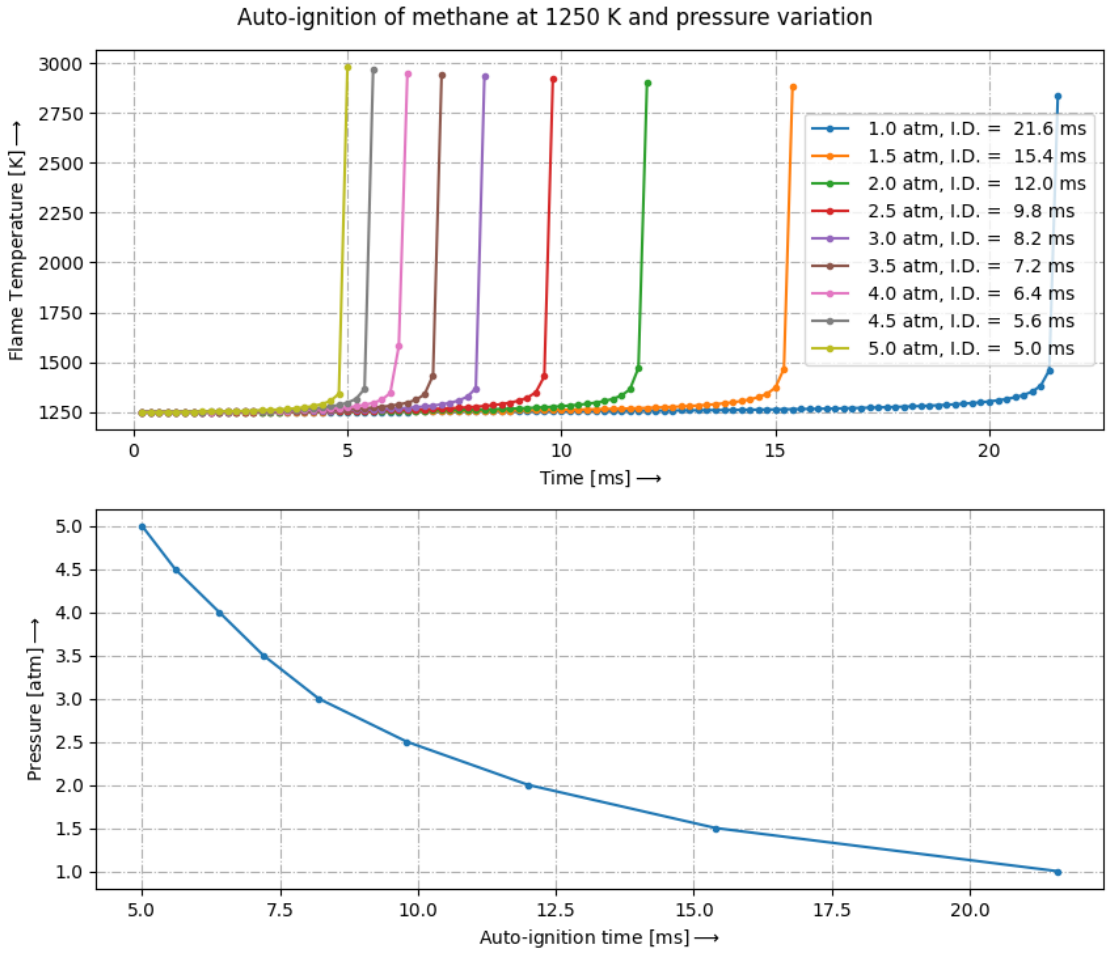

Figure 1: Influence of pressure

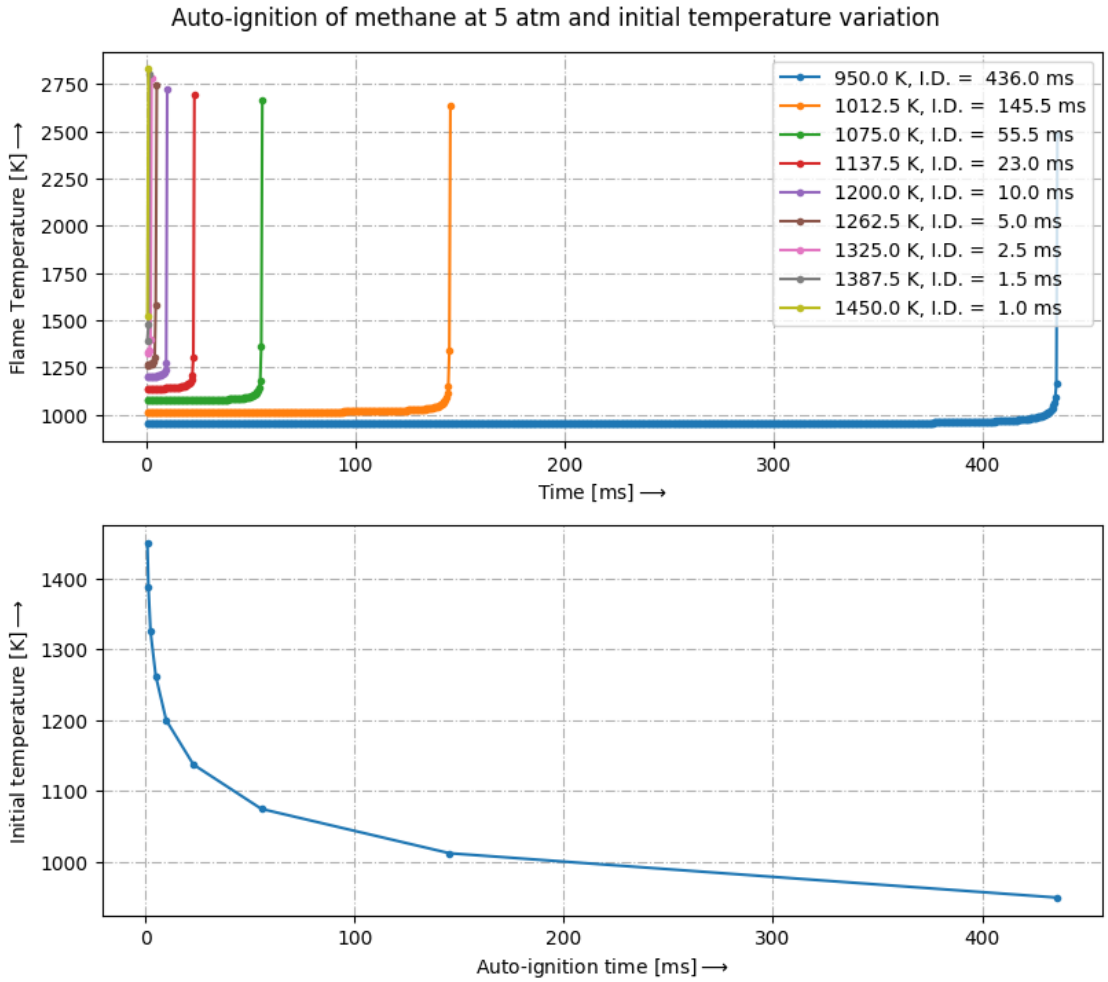

Figure 2: Influence of temperature

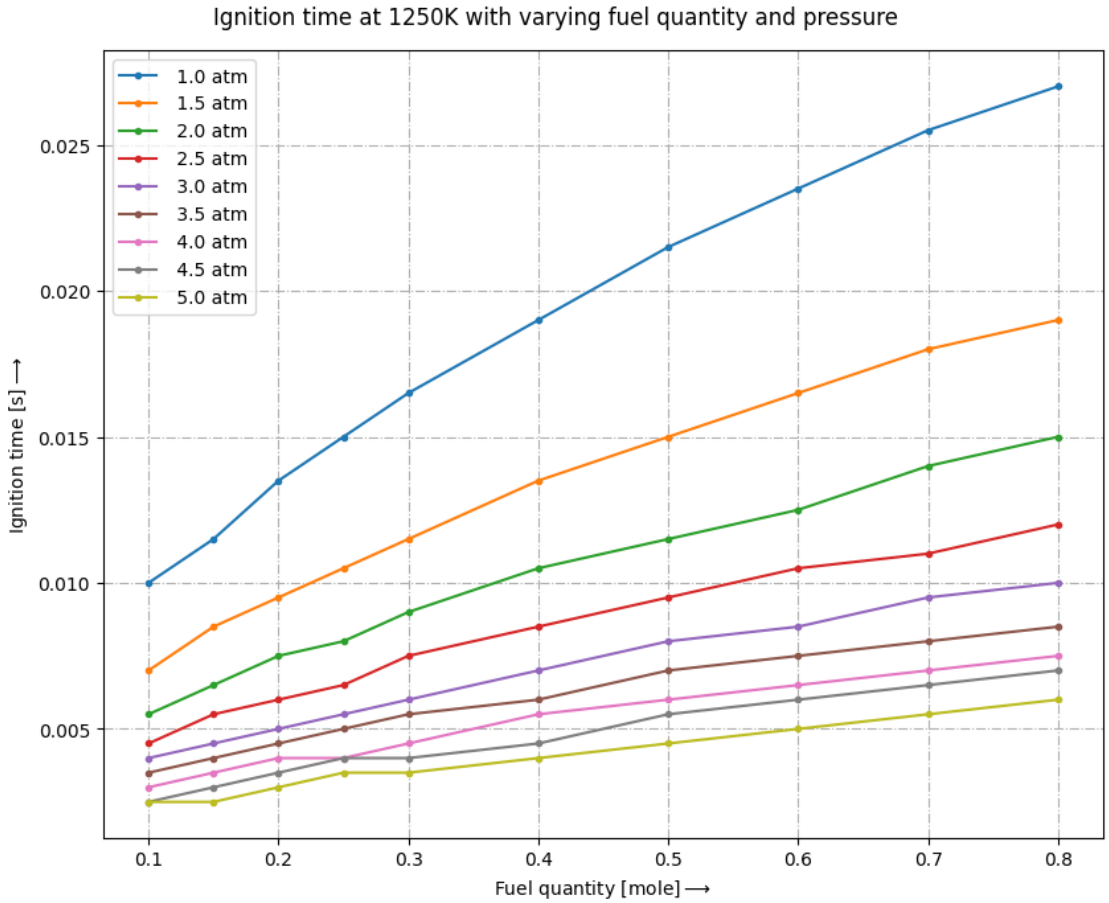

Figure 3: Influence of pressure and molar composition

4 Conclusions

1. Regarding the effect of pressure on ignition delay, it was observed that higher pressures generally lead to shorter ignition delays. This can be attributed to greater collision frequency. As the pressure increased, the speed of the reaction increased, thus making the combustion happen earlier.

2. The same conclusion can be drawn upon the mixture's initial temperature. Again, higher temperatures resulted in faster ignitions. As trivial as it may sound, higher temperatures can therefore be associated with higher thermal energy, and thus, as can be observed, they cause more violent reactions.

3. Lastly, varying the molar composition of the fuel mixture revealed a noteworthy impact on the autoignition time. At the conditions applied, the ignition generally did not happen earlier for higher methane condensations, as it could have been anticipated. That is due to the fact that the amount of oxygen was constant throughout all the simulations and was not increased correspondingly.

In conclusion, the simulations conducted within the project are in accordance with fundamental laws of physics, accurately modeling the phenomenon of combustion of

methane. Moreover, they exhibit consistency among themselves - i.e. the ignition times for case 2 are similar to the ones in case 3 for 0.8 moles of methane (the closest to 1 - stoichiometric reaction). The investigation into the relationship between pressure, temperature, molar composition, and ignition delay provides valuable insights into the autoignition behavior of methane.

5 References

'Simulating auto ignition using Cantera', Kshitiz Sahai

https://github.com/msienicki/Projekt-Cantera-Mateusz-Sienicki