INFLUENCE OF INITIAL PRESSURE AND TEMPERATURE ON HYDROGEN-OXYGEN MIXTURES' IGNITION DELAY TIME

Computational methods of combustion

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1 INTRODUCTION

Purpose of this project is to evaluate the relation between the ignition delay time and initial conditions such as temperature and pressure for various hydrogen-oxygen mixtures. The simulations were performed using Cantera package for Python.

Ignition delay time is an important parameter of a combustible mixture. It tells how long it takes for a mixture to ignite, after suitable conditions (e.g. temperature) are met. One of its exemplary appliances lies in detonation theory - the distance between the shockwave and the flame front can be easily calculated using ignition-delay time.

2 METHODS

2.1 Model

Model consists of a constant-volume reactor (cantera.IdealGasReactor with gri30 reaction mechanism) filled with a combustible mixture with given initial pressure, temperature and concentration. The ignition-delay time is defined as follows:

$$\Delta t = t_i - t_0 \tag{1}$$

Where: Δt - ignition delay time, t_i - time of ignition, t_0 - reference time, e.g. simulation starting time.

t_i is determined by the concentration of hydrogen radicals (H). The exemplary plot is shown on figure 2. For the purpose of this project, t_i is defined as the moment of maximum concentration of H.

2.2 Code description

The core of the simulation is a function, which takes pressure, temperature and composition as parameters and returns the ignition-delay time. It creates all the necessary cantera objects (Solution, IdealGasReactor, ReactorNet) and performs the simulation step by step in a loop. In each iteration the level of hydrogen radicals is monitored. If it is not smaller than in the previous step, the simulation continues. If not, the maximum concentration has been reached and the loop stops and the current time is returned. If no ignition has been reached in 0.01 s, further calculations are stopped and the function returns -1.

Calculations were performed for pressure range of 0.2 to 10 atm and temperature range of 1200 to 3000 K.

3 RESULTS

Figure 1 shows the relation between ignition time and stoichometric ratio. Initial conditions were: $T = 1500K$ and $P = 10atm$. As can be seen minimal ignition time occurs around stoichiometric conditions.

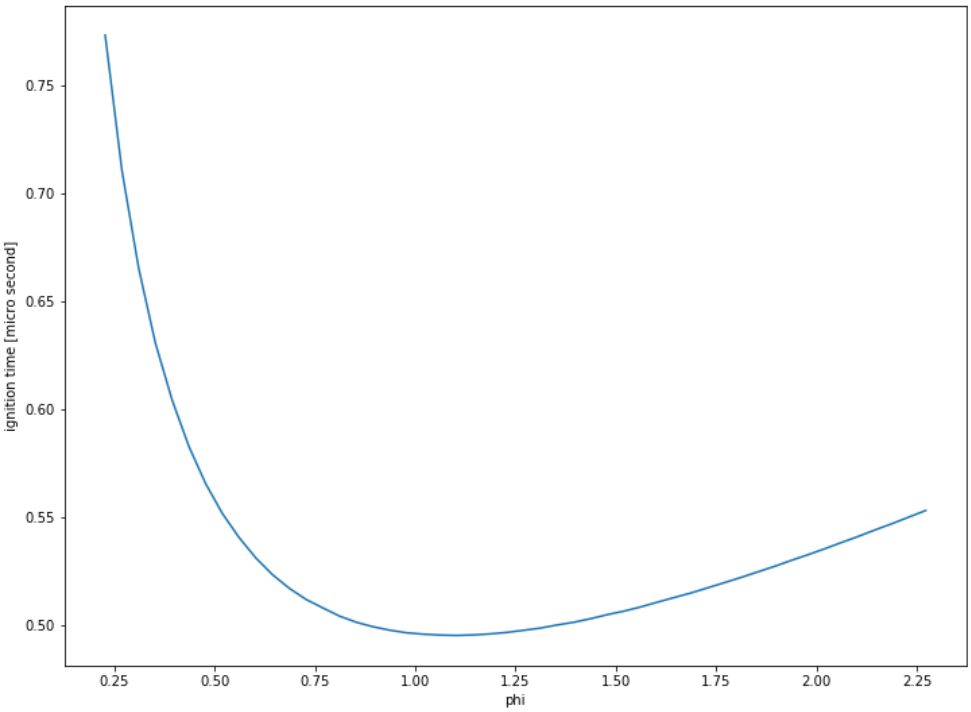


Figure 1: Relation between ignition time and stoichometric ratio.

Figure 3 shows time course of concentration of hydrogen radicals.

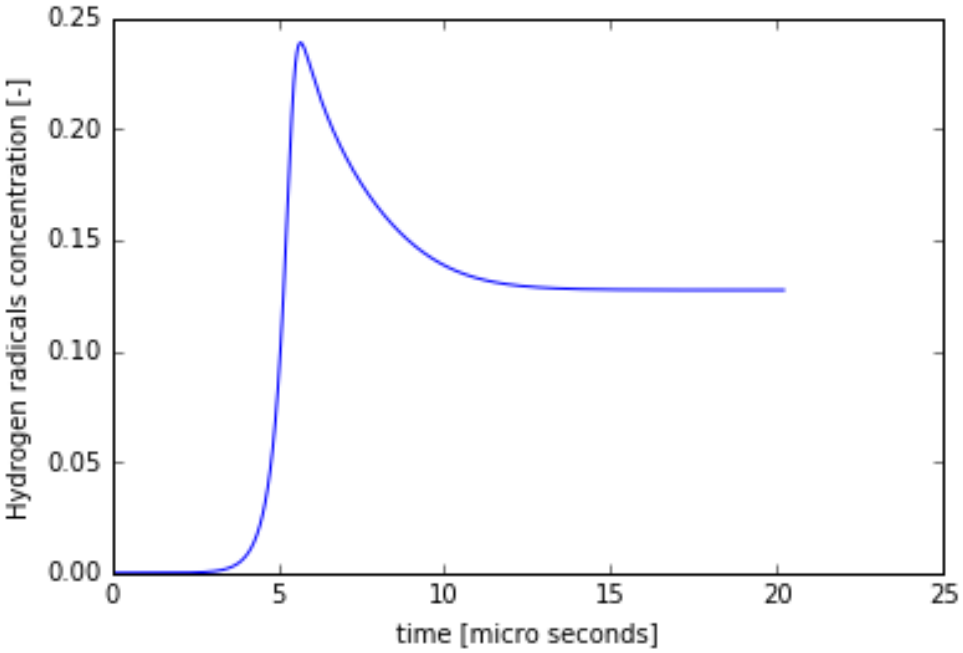
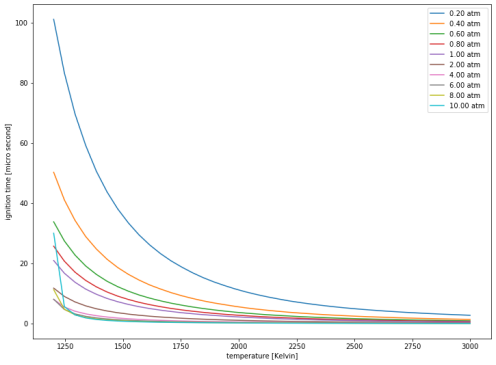
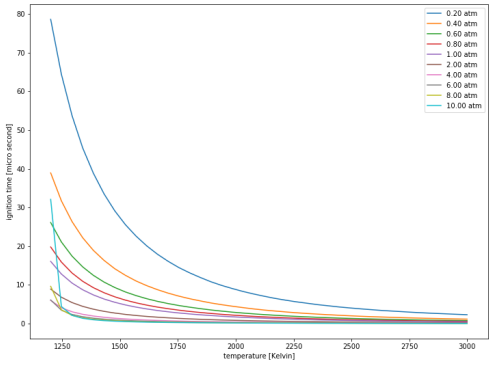


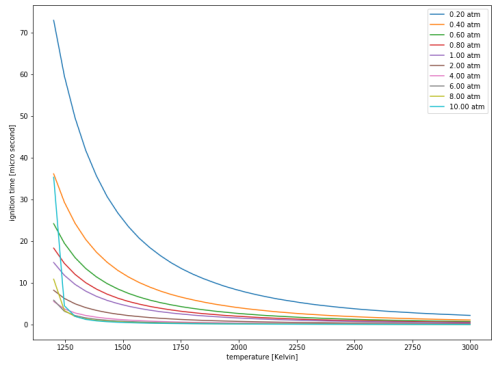
Figure 2: Time course of concentration of radicals



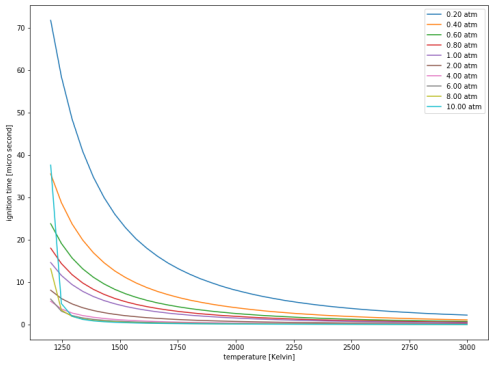
(a) $\phi = 0.23$



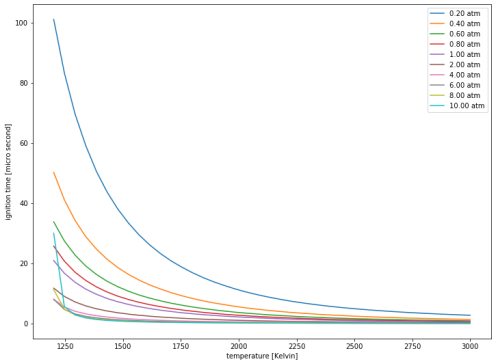
(b) $\phi = 0.47$



(c) $\phi = 0.72$



(d) $\phi = 1$



(e) $\phi = 1.2$

Figure 3: Ignition time for various initial conditions (temperature and pressure)

4 SUMMARY

As shown above ignition time is a parameter highly dependent on initial mixture conditions. The ways with which it's value can be reduced are:

1. Combustion near stoichiometric conditions
2. Increasing mixture initial temperature

3. Increasing mixture initial pressure

REFERENCES

[1] Cantera
http://www.cantera.org/docs/sphinx/html/index.html