Computational methods of combustion

Influence of initial temperature and pressure on methane oxygen mixtures' ignition delay time

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1. Introduction

The purpose of this project is to conduct a series of simulations for various methane oxygen mixtures and show the relation between ignition delay time of the said mixture and initial temperature as well as initial pressure. The simulations were performed using Cantera package in Python.

2. Definition

Ignition delay time (henceforth it will be referred to as IDL) is an important parameter in combustible mixtures, as it shows how long does it take for a mixture to ignite after having reached the suitable conditions. Early determination of the autoignition characteristics of any combustible mixture provides substantial information for combustion systems development.

3. Mathematical model

The autoignition time has been determined by using temperature gradient i.e., the time of the sharpest increase of temperature being the autoignition point. The methane oxygen mixture was put in a constant volume reactor. Then all the necessary parameters for the calculation of IDL were set.
The basis of the function is quite simple: it takes temperature, pressure and mixture composition in, performs the simulation and returns IDL instead. In order to determine IDL more accurately the time step of 10^-6 s has been chosen.
Calculations were performed for temperature and pressure range of 1000K to 2000K and 1atm to 4atm respectively.

4. Results

Figure 1 shows the correlation between initial temperature and ignition delay time for p = 1 atm, and mixture composition $\phi = 1$.

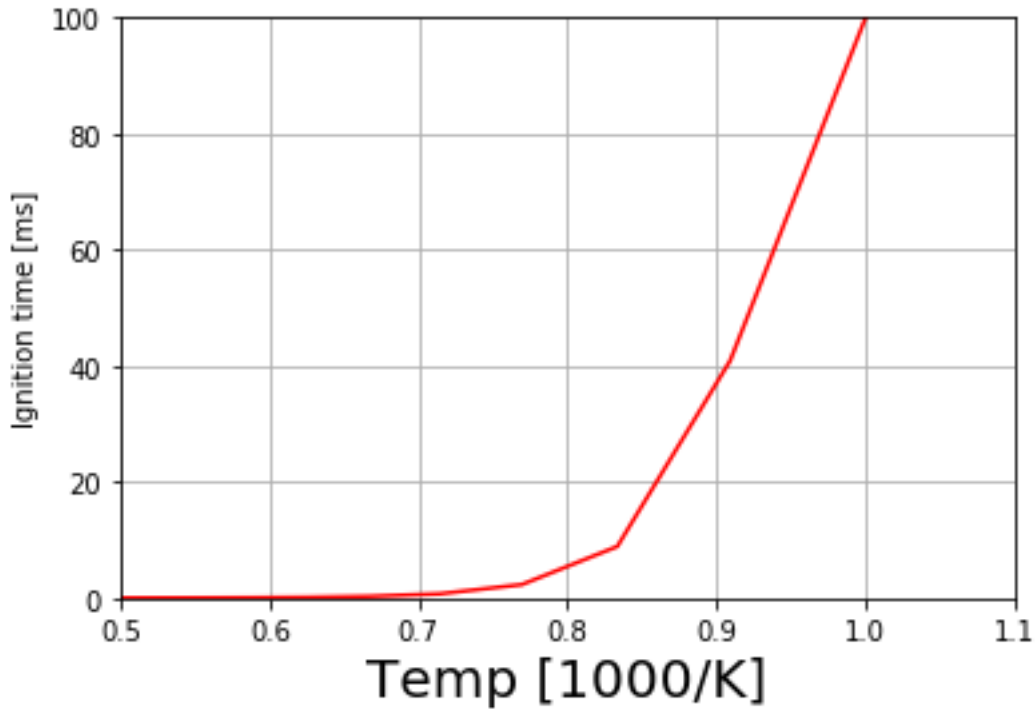

Figure 1. IDL dependence on initial temperature

Ignition delay time decreases for higher initial temperature. Autoignition does not occur below certain value of temperature, T = 1100 K in this case.

Figure 2 shows the correlation between ignition delay time and initial pressure for T = 1200 K and $\phi = 1$.

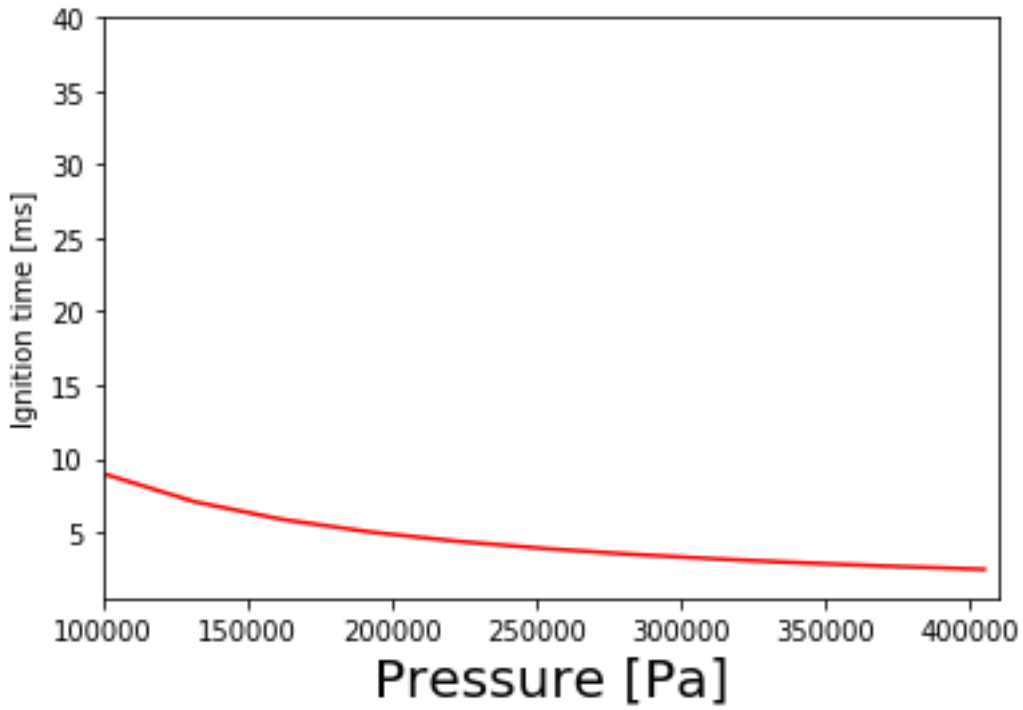

Figure 2. IDL dependence on initial pressure

Ignition delay time decreases for higher pressure values.

5. Conclusion

a) Ignition delay time as can be seen above is determined by the initial mixture condition.
b) Ignition delay time can be reduced by: increasing initial mixture temperature or initial mixture pressure.

6. References.

http://cantera.org/docs/sphinx/html/cython/examples/reactors_combustor.html

https://arxiv.org/pdf/1706.01987.pdf