Combustion parameters of ethene-air mixture

Computional methods in combustion

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1 Introduction

The aim of this project was to show how composition of fuel-air mixture, as well as its initial temperature and pressure influences the time of auto-ignition, maximum pressure and temperature. The simulation was conducted using "Cantera" package and reaction mechanism called "GRI-Mech 3".

2 Model

In order to simulate auto-ignition, the reactor mechanism of Cantera was used and following assumptions were made:

- The fuel was perfectly mixed with air
- The air consisted only of oxygen and nitrogen in 1:3.76 ratio
- Reactor's walls were non-conductant and non-reactive

The stoichometric reaction of complete combustion of ethene in air:

$$C_2H_4 + 3O_2 + 11.28N_2 \longrightarrow 2CO_2 + 2H_2O + 11.28N_2$$

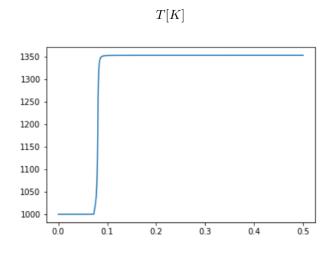
Calculations were performed for various initial parameters

3 Results

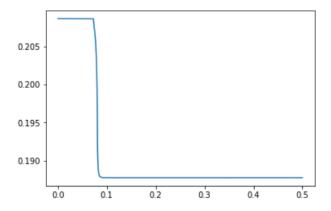
3.1 Variable equivalence ratio

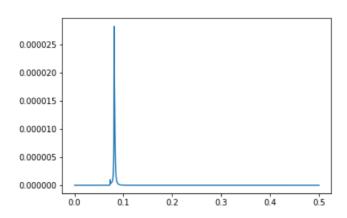
$$T_0 = 1000K, p = 101325Pa$$

3.1.1 $\phi = 0.1$

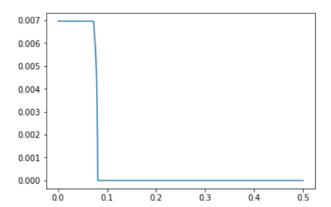


$O_2 content$

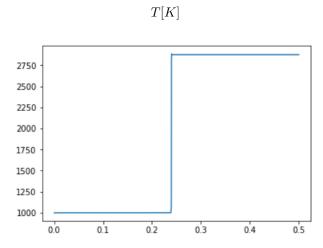




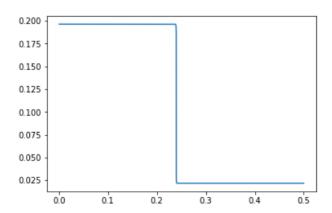
 $C_2H_4content$

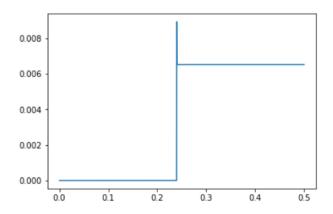


3.1.2 $\phi = 1$

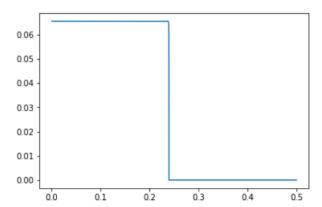




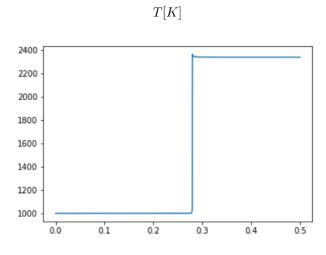




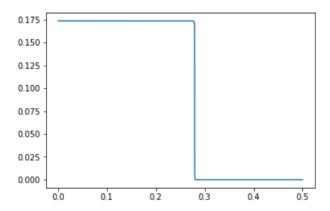
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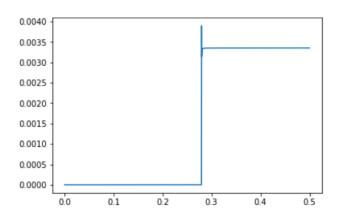


3.1.3 $\phi = 3$

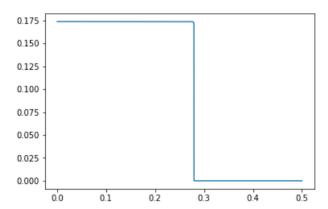








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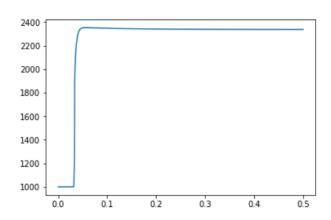


3.2 Variable initial pressure

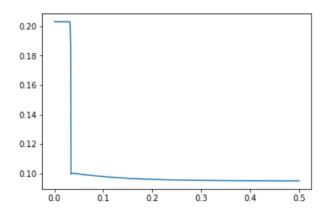
$$\phi = 0.5, T_0 = 1000K$$

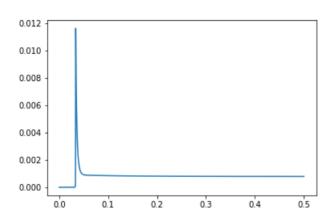
3.2.1 *p*=**10000Pa**

T[K]

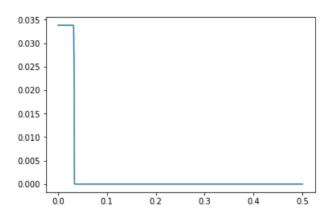


$O_2 content$

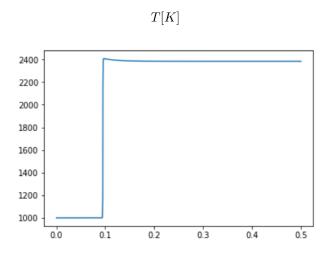




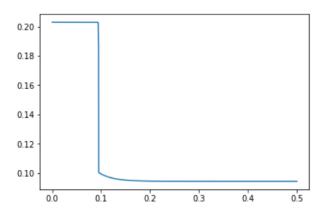
 $C_2H_4content$

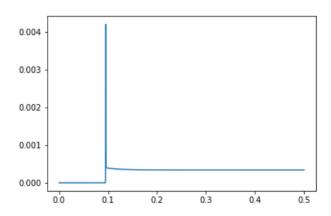


3.2.2 *p*=**50000Pa**

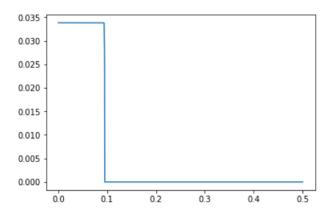


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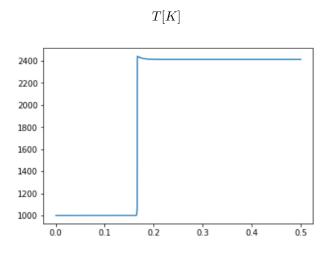




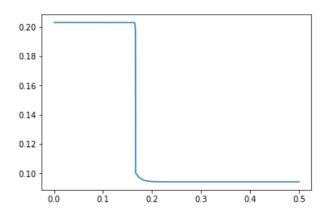
 $C_2H_4content$

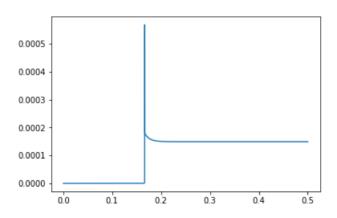


3.2.3 *p*=**200000Pa**

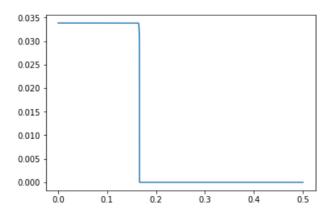








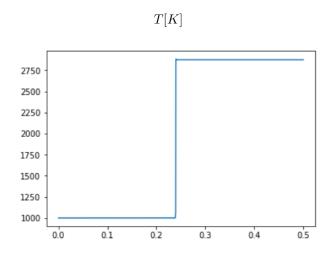
 $C_2H_4content$



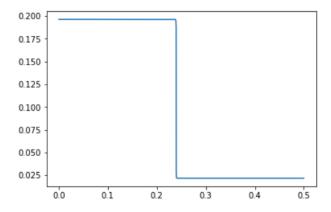
3.3 Variable initial temperature

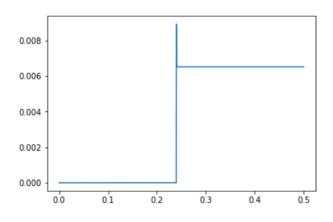
$$\phi=1, p=101325Pa$$

3.3.1 $T_0 = 1000 \text{K}$

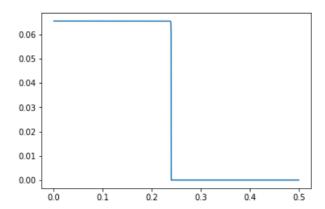








 $C_2H_4content$

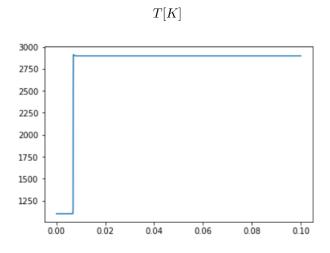


3.3.2 $T_0 = 1100 \text{K}$

0.200 0.175 0.150 0.125 0.100 0.075 0.050

0.00

0.02



 $O_2 content$

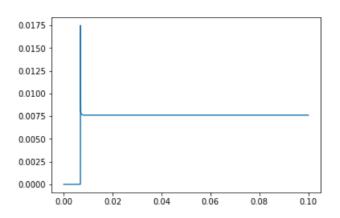
0.04



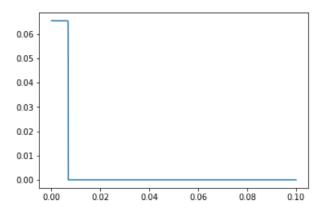
0.06

0.08

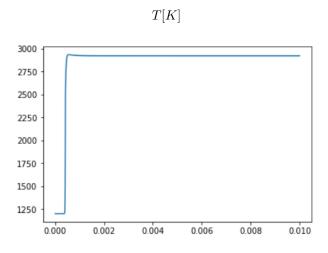
0.10



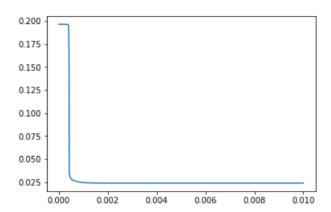
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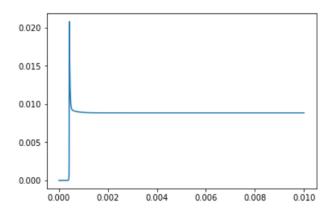


3.3.3 $T_0 = 1200 \text{K}$

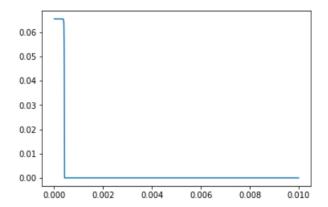








 $C_2H_4content$



all charts are in function of time $[\mathbf{s}]$

4 Summary

The results were as expected; higher initial temperatures resulted in shorter auto-ignition times and the highest temperature was achieved with stoichiometric composition on mixture ($\phi = 1$).

The study was a valuable introduction to both "Cantera" package as well as to "LaTeX" software.