Auto-ignition of ethane-air mixture

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1 Introduction

This project will be dedicated to a simulation of auto-ignition ethane-air mixture with different starting parameters, which are: temperature, pressure and equivalence ratio. The purpose is to analyze if auto-ignition starts and if it does, then to get to know time after which the phenomena occurs.

2 Auto-ignition definition

Auto-ignition is a spontaneously ignition of the fuel - oxidizer mixture without the presence of a flame. One of the most important parameter is the auto-ignition temperature, which define absence of this phenomenon. Below this temperature the auto-ignition does not occur. Mostly it depends on composition and pressure of the flammable mixture.

3 Mathematical model

In closed generated reactor will be hold a simulation of mixture evolution under specific conditions until it will reach its equilibrium state. Calculations will be conducted one-hundred-thousand times with time step dt=10e-6 for each step of temperature, pressure and equivalence ratio. Auto-ignition point is the one with the highest temperature gradient.

4 Mathematical calculations of equivalence ratio

Chemical stoichiometry needed to find the equivalence ratio:

$$2C_2H_6 + 7(O_2 + 3.76N_2) = 4CO_2 + 6H_2O$$

$$(F/A)_{stoichiometric} = \frac{2}{7(1+3.76)} = 0.060024$$

$$\phi = \frac{F/A}{(F/A)_{stoichiometric}}$$

$$F/A = \phi * (F/A)_{stoichiometric}$$

$$A = \frac{F}{\phi * (F/A)_{stoichiometric}}$$

In the program I will assume constant number of ethane moles, so only amount of air moles will be changing according to the equation above.

5 Boundary parameters used in the project

$$T_{min} = 1100K$$
$$T_{max} = 2400K$$
$$P_{min} = 1atm$$
$$P_{max} = 3atm$$
$$\phi_{min} = 0.4$$
$$\phi_{max} = 3.4$$

6 Results

Program returns charts of final temperature and auto-ignition time in relation with one of variables, which are: equivalence ratio, initial temperature and pressure. Program saves all of results to the .csv format file.

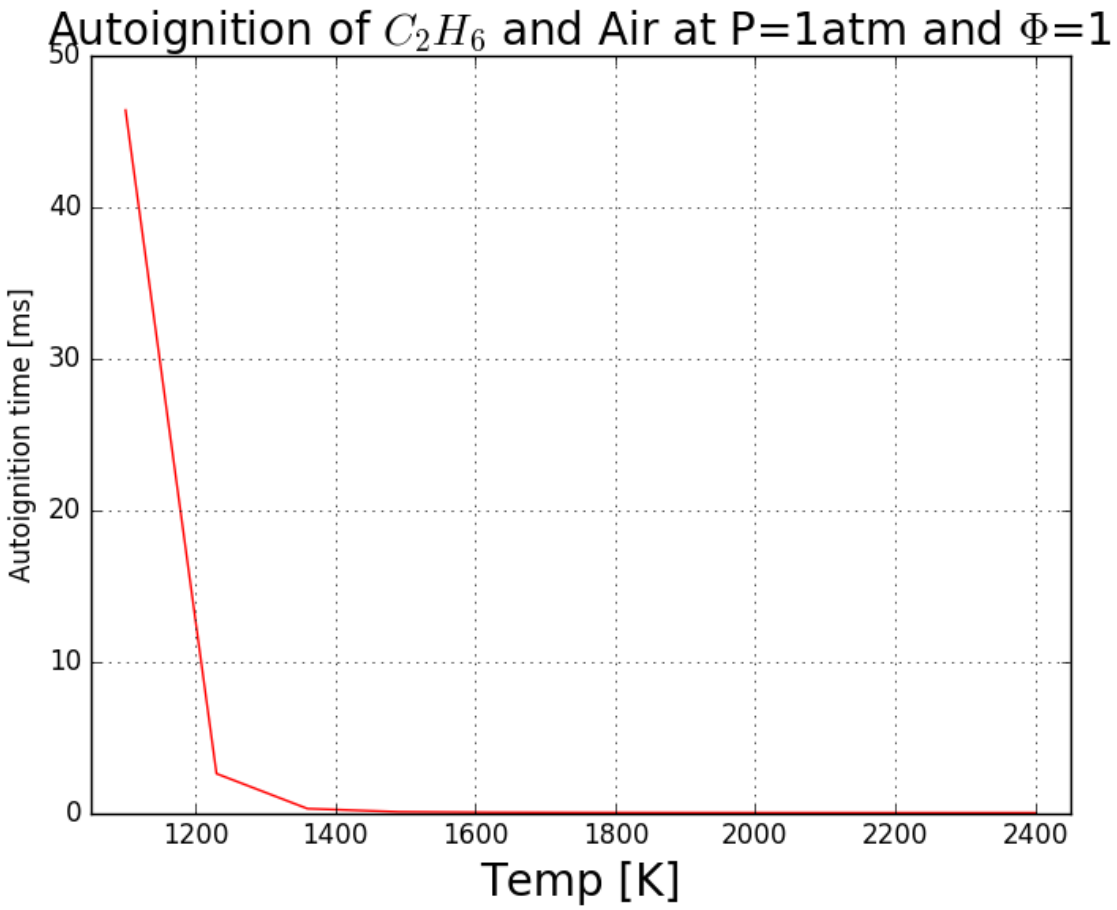

Figure 1: Time of self-ignition drastically diminish, what means that minimal initial temperature used in the project is close to the temperature, below which auto-ignition does not occur.

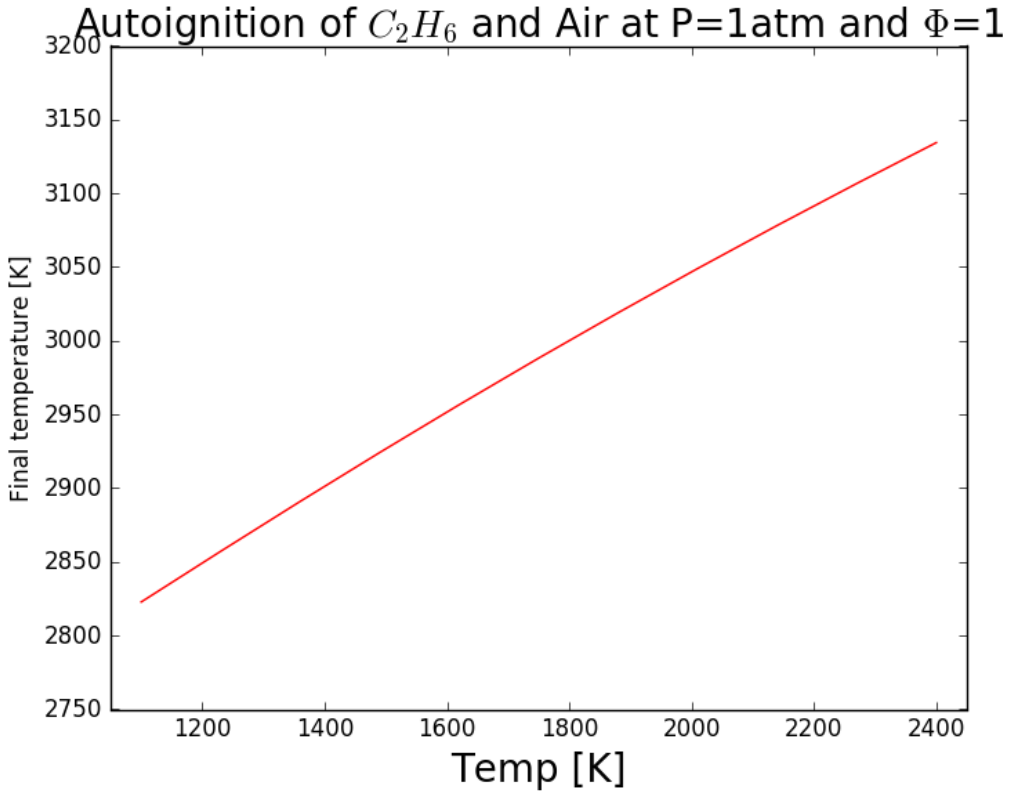

Figure 2: Graph above presents almost linear function. Value of the final temperature is growing with increase of the initial temperature

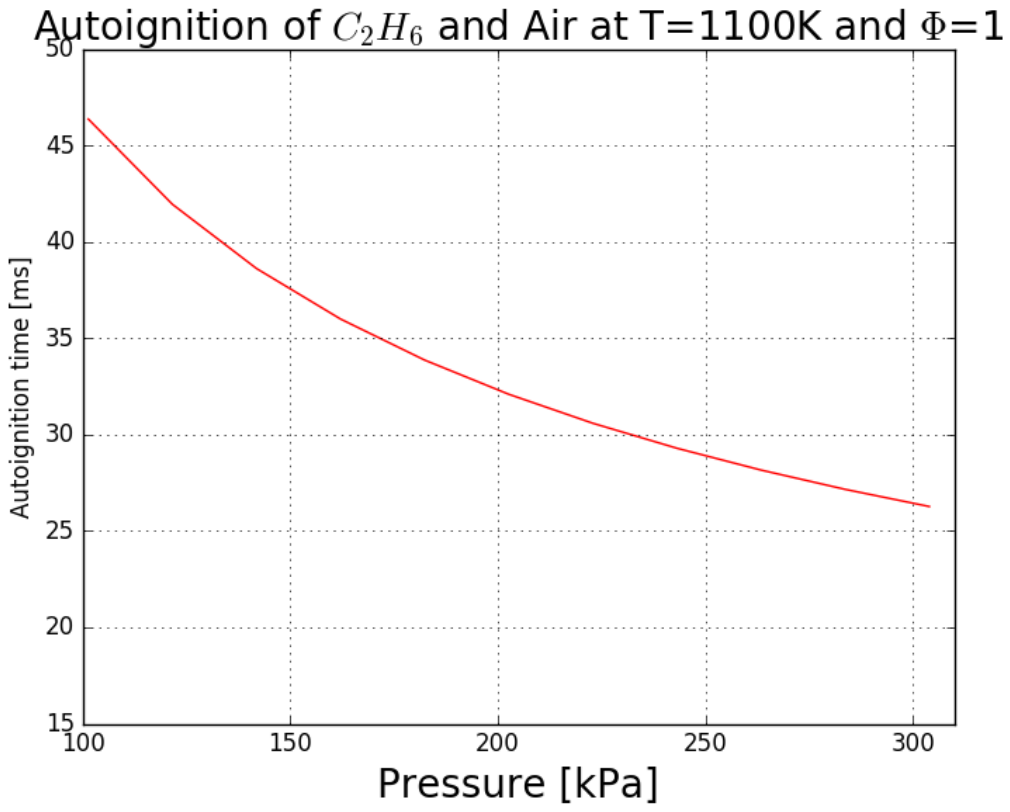

Figure 3: By tripling the pressure self-ignition happens twice times faster. Function's gradient gets smaller with growing pressure.

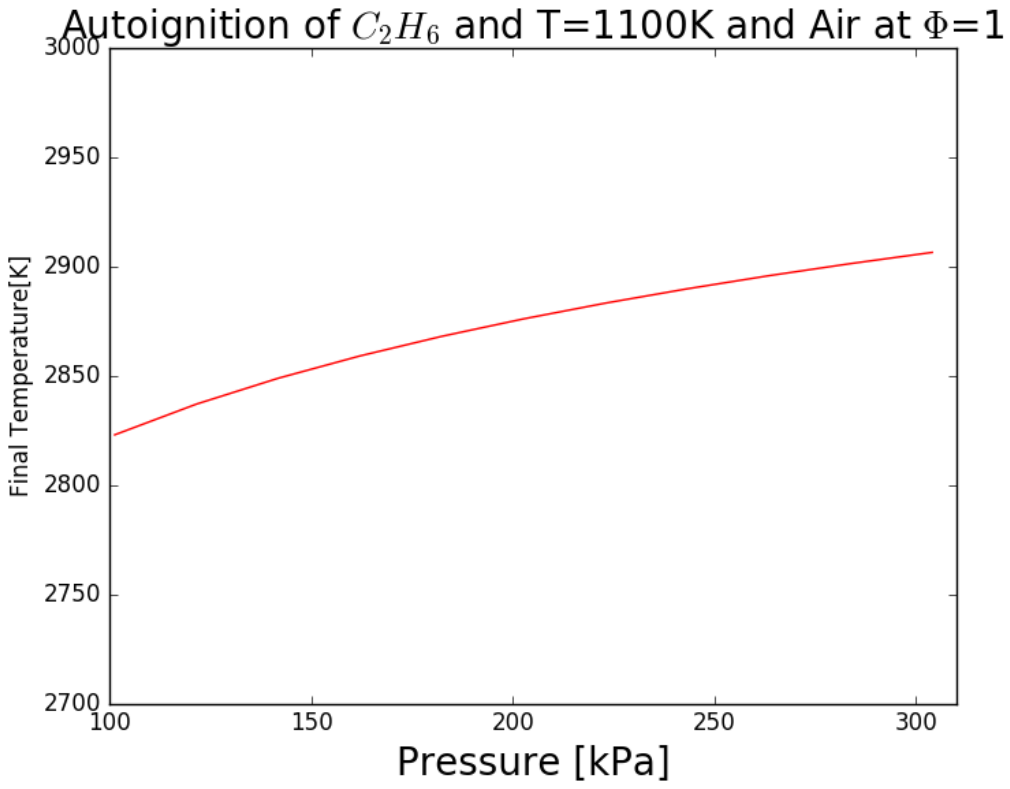

Figure 4: Final temperature grows up with increasing pressure, whatsoever pressure does not have as big influence on the final temperature as two other parameters.

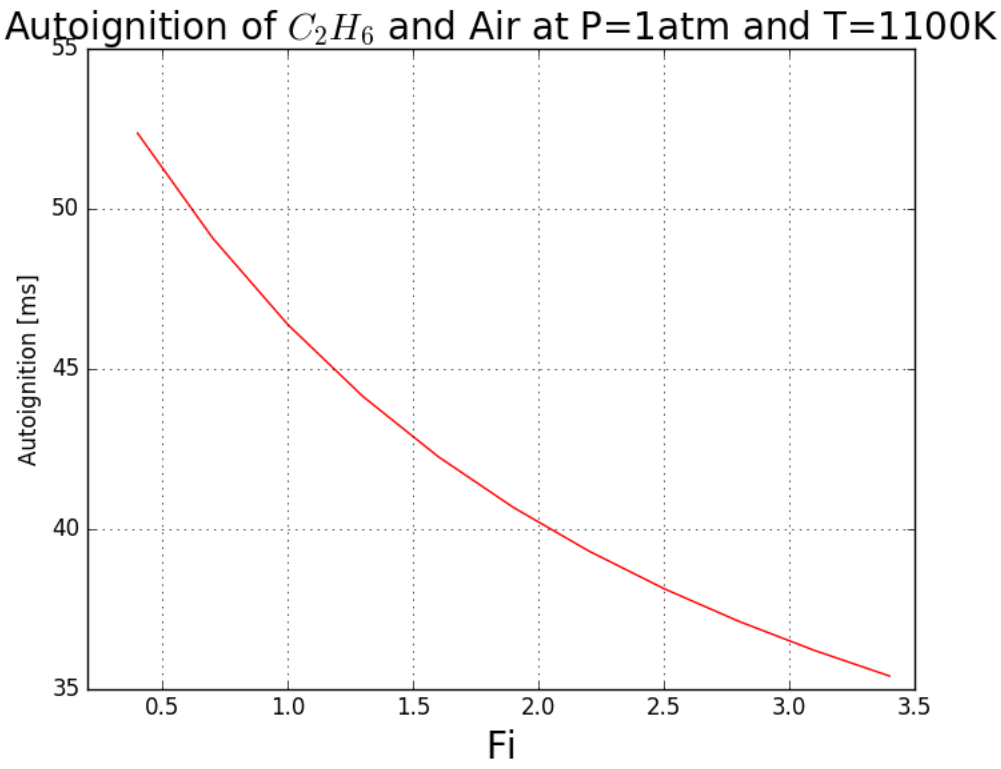

Figure 5: By increasing Fuel to Air ratio, auto-ignition time is decreasing. Gradient gets smaller with growing ϕ.

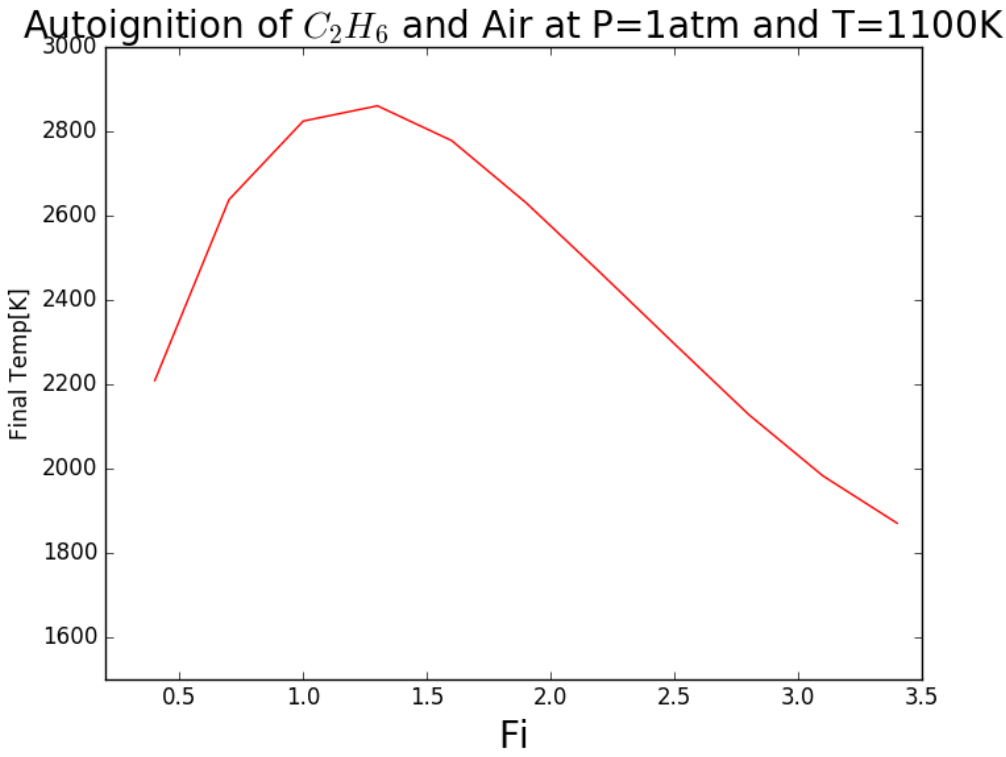

Figure 6: Fi parameter seems to be most significant for final temperature function cause of its characteristics. It reaches its maximum for Fi = 1.3 and FinalTemp = 2856 K

7 Conclusions

All of the simulations of burning fuel and others are crucial for choosing most beneficial parameters during tests. In self-ignition simulation described in this document we could observe: increasing parameters of initial pressure and initial temperature result in lowering self-ignition time and rising final temperature; for growing Fi, even though decreasing auto-ignition time, we can notice huge growth and huge minimize of the final temperature after specific point.

8 References

[1]*CANTERAHandsOn.pdf*