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Metody komputerowe w spalaniu
Projekt Cantera

Prowadzący:
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1. Introduction

This raport contains summary of combustion of propane in mixture with air with certain properties. General assumption is to simulate combustion process that happens inside of 4-stroke internal combustion engine, where fuel is LPG.
Calculations were carried out using Cantera - open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes. Reactor object with Cantera will be prepared to determine the auto-ignition timing of a mixture, and observe changes of temperature, pressure, and content of certain chemical elements in created mixture.

2. Literature/ internet sources

For internal combustion engine information a book was used:

- Tłokowe silniki spalinowe - Jan A. Wajand; Jan T. Wajand; Wydawnictwo Naukowo-Techniczne [1]

Other information on combustion process in engine internet sources were used:

- https://en.wikipedia.org/wiki/Liquefied_petroleum_gas [2]
- https://en.wikipedia.org/wiki/Propane [3]
- https://sites.google.com/site/silnikipojazdowsamochodowych/ [4]
- https://www.elgas.com.au/blog [5]

And sites used for python-cantera code generation:

- https://cantera.org/examples/python/reactors/ [6]
- Chapter 4 from Cantera tutorials pdf: https://www.cerfacs.fr/cantera/docs/tutorials/CANTERA_HandsOn.pdf [7]
- https://cantera.org/science/reactors.html [8]

Also some private sources on internal combustion engines (from other engine-related subjects).

3. Model description

LPG is a mixture of 2 hydrocarbon gases - propane and butane, in several percentage combinations. Because in this case GRI-Mech 3.0, the 53-species, 325-reaction natural gas combustion mechanism is used, I decided to simplify calculation by using only propane - which is available in this database.
gas1 = ct.Solution('gri30.xml')

2 models were prepared - first one with complete combustion of propane is presented and second with incomplete, the actual model of combustion that occurs inside of combustion chamber for 4-stroke internal combustion engine.
Here are chemical processess that happen:
1) complete combustion:

$$C_3H_8 + 5O_2 + 18.8N_2 \rightarrow 3CO_2 + 4H_2O + 18.8N_2 + Heat$$

2) incomplete combustion:

$$C_3H_8 + 4{,}5O_2 + 16.92N_2 \rightarrow 2CO_2 + CO + 4H_2O + 16.92N_2 + Heat$$

In both cases, of course propane reacts with air (which is assumed to be mixture of oxygen and nitrogen in ratio 1:3,76 - air consists 21% of O_2 and 79% of N_2, other gases are omitted).
In complete combustion carbon dioxide and water are products, heat is generated.
In incomplete carbon dioxide, carbon monoxide and water are products, heat is generated.
Carbon monoxide is generated when not enough oxygen is present in reaction, it is popular "soot" that settles on the cylinder, pistons and other engine elements.
So it is important to control engine parameters to avoid that situation - like moment of ignition, ratio of LPG to air and so on.
Properties of LPG-air mixture inside of combustion chamber of of four-stroke internal combustion engine found in internet& literature - max pressure (shortly before combustion) is around 3MPa. In theory temperature of propane autoignition is equal to around 490 Celsius degree= 763 K, but this is information for atmosferical pressure (101325 Pa) which does not occur in that case. Time of propane combustion inside of an engine should be around 0.001s. Temperature inside of combustion chamber is around 2500-3000 Celsius degree after fuel is burned; initially, before combustion process it should be around 900 Celsius degree.
T = 1200
P = 3000000
X = 'C3H8:1 O2:4.5 N2:16.92'
gas1.TPX = T,P,X

So values putted into simulation are: T=1200K, P=3MPa, with gases and it's ratios explained above:

```
gri30:

       temperature             1200   K
          pressure            3e+06   Pa
           density          8.87933   kg/m^3
  mean mol. weight          29.5307   amu

                          1 kg             1 kmol
                       -----------      ------------
          enthalpy      9.5858e+05        2.831e+07     J
   internal energy      6.2072e+05        1.833e+07     J
           entropy            7599        2.244e+05     J/K
```

```
   Gibbs function      -8.1602e+06        -2.41e+08     J
heat capacity c_p           1387.9        4.099e+04     J/K
heat capacity c_v           1106.4        3.267e+04     J/K

                             X                 Y          Chem. Pot. / RT
                    -------------     -------------     -------------
               O2        0.200714          0.217488          -25.3049
               N2        0.754683          0.715908          -22.2366
             C3H8        0.044603         0.0666031          -51.3808
     [   +50 minor]             0                 0
```

Next thing, after [7] is to fill reactor with created gas and prepare a ReactorNet object:
r=ct.Reactor(gas1)
sim=ct.ReactorNet([r])

To be able to prepare plots arrays to hold data have to be prepared:
times = np.zeros(1000)
data = np.zeros((1000,5))
We will look at temperature (0), pressure (1) and contents of O_2, H and C_3H_8 (2,3,4) throughout time of simulation.

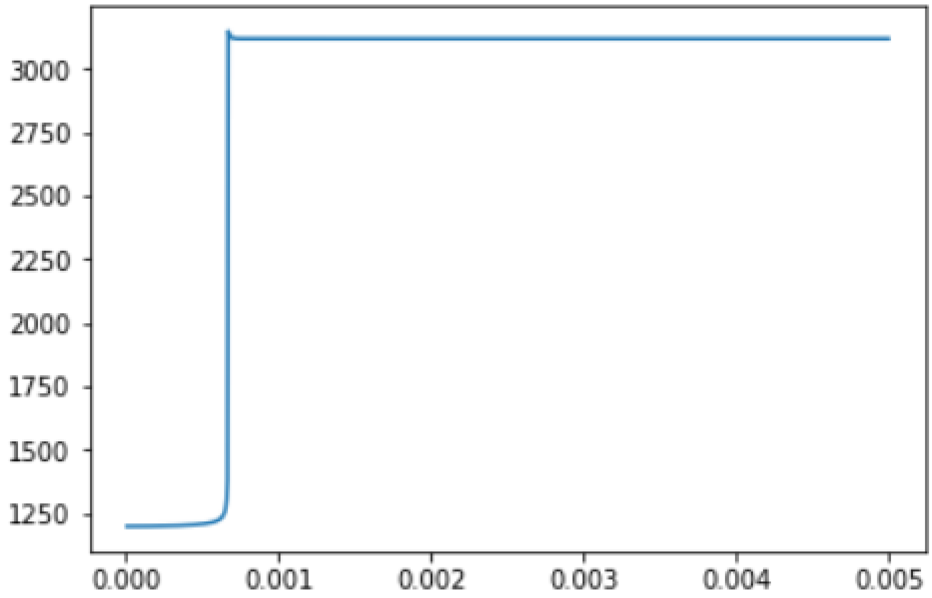
Some parameters used to create data have to be defined (time - start time of simulation; tf - end time of simulation; dt - timestep; n- initial value of n in loop):
time=0
tf = 0.005
dt=tf/1000
n=0
I decided to divide whole simulation by 1000, to get 1000 data points.

Loop for plots creation is created using for command:
for n in range(1000):
time += dt
sim.advance(time)
times[n] = time
data[n,0] = r.T
data[n,1] = r.thermo.P
data[n,2:]=r.thermo['O2', 'H' , 'C3H8'].X

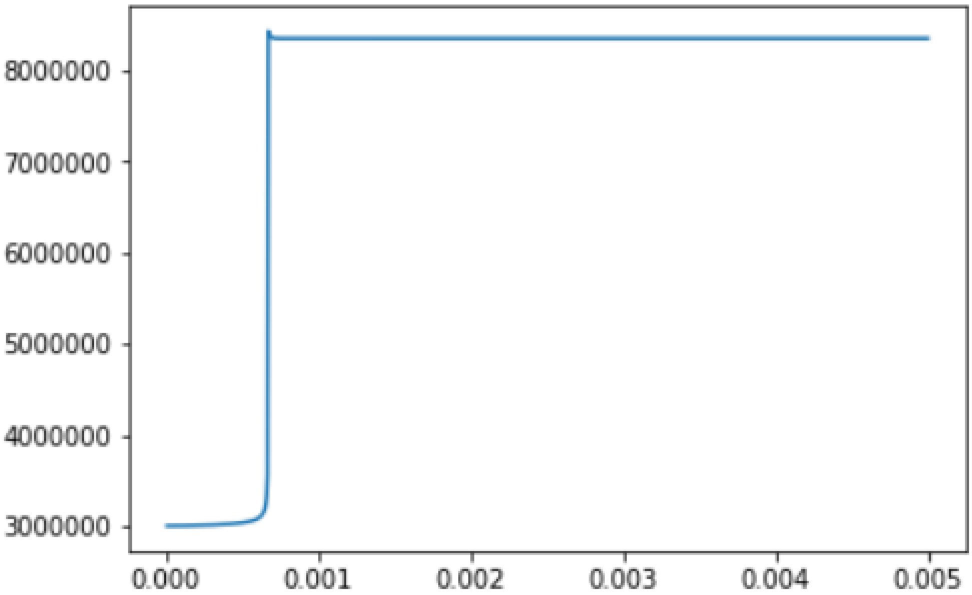
Last thing in entire code is to print out previously mentioned plots with command (presented is for temperature in simulation vs time):
plt.plot(times,data[:,0])
plt.show()

4. Results description

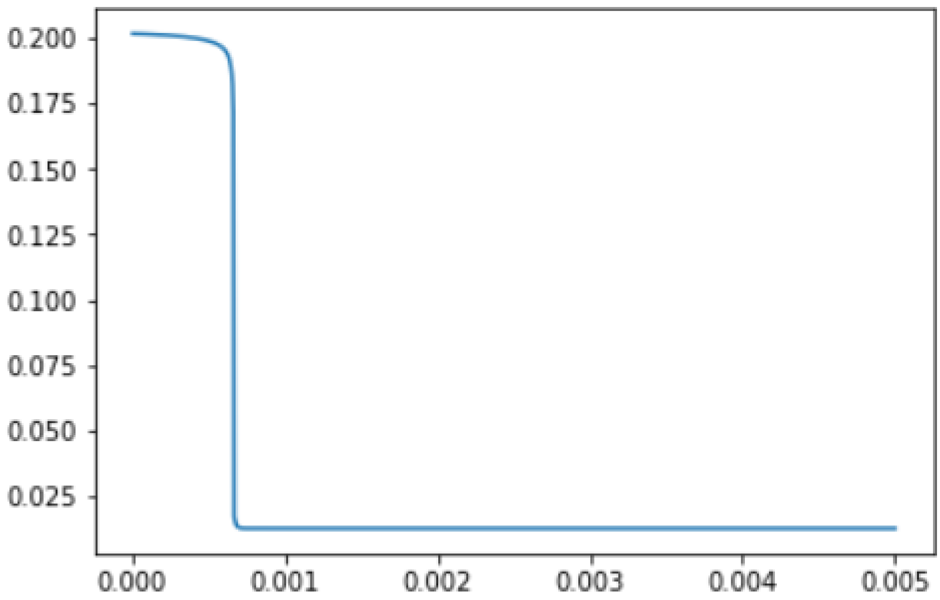
4.1. Complete combustion case



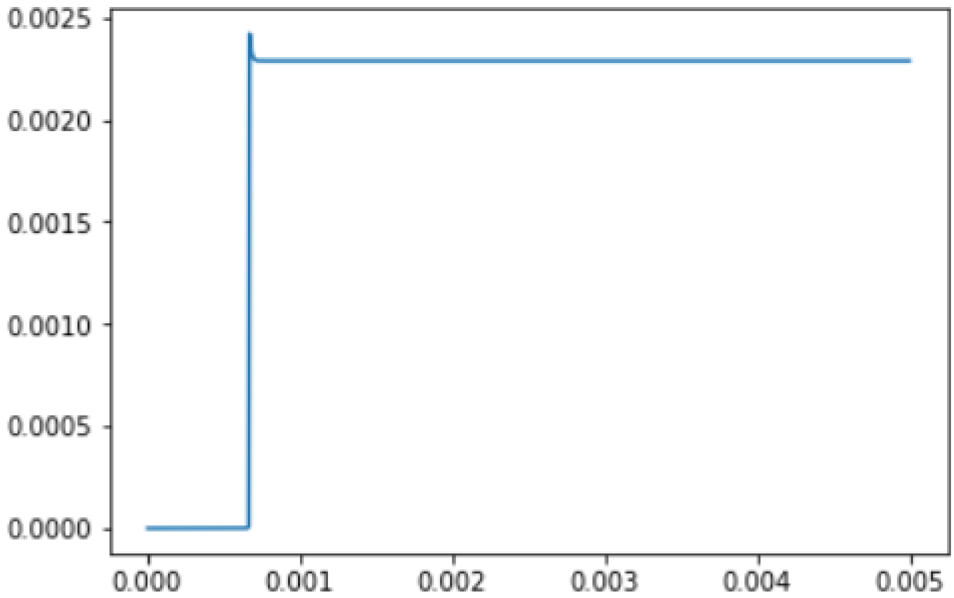
4.1.1. Temperature vs time of simulation for complete combustion case



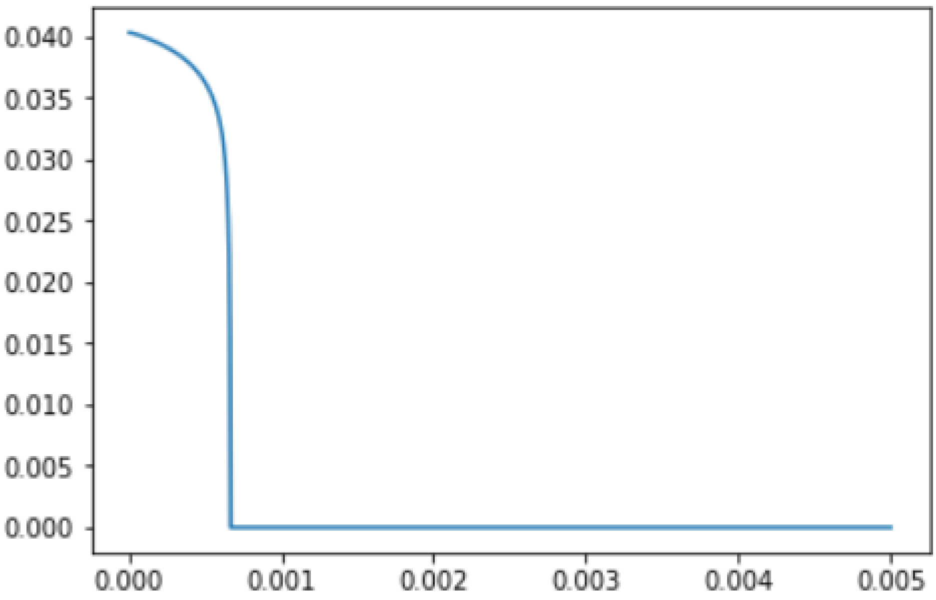
4.1.2. Pressure vs time of simulation for complete combustion case



4.1.3. Oxygen content vs time of simulation for complete combustion case

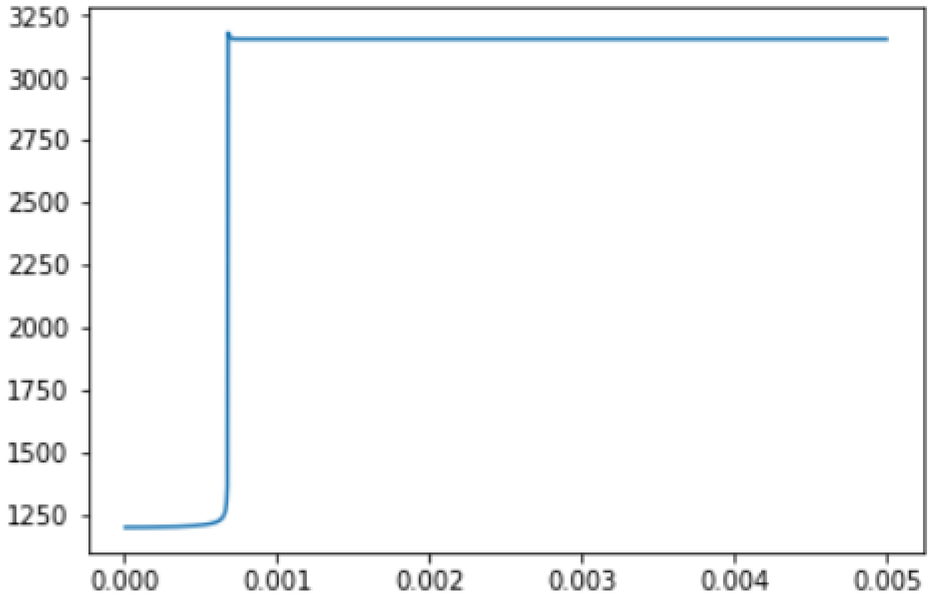


4.1.4. Hydrogen content vs time of simulation for complete combustion case

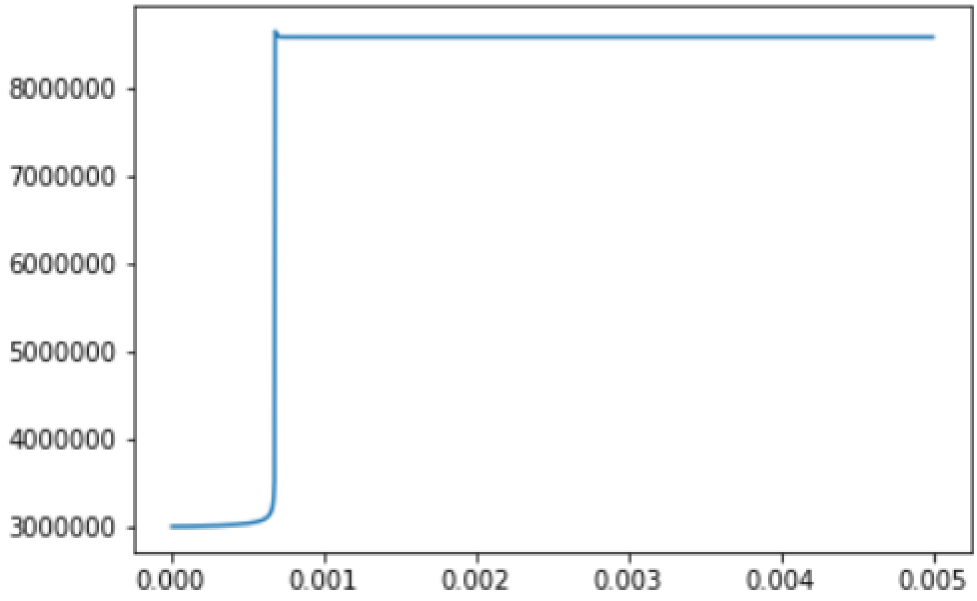


4.1.5. Propane content vs time of simulation for complete combustion case

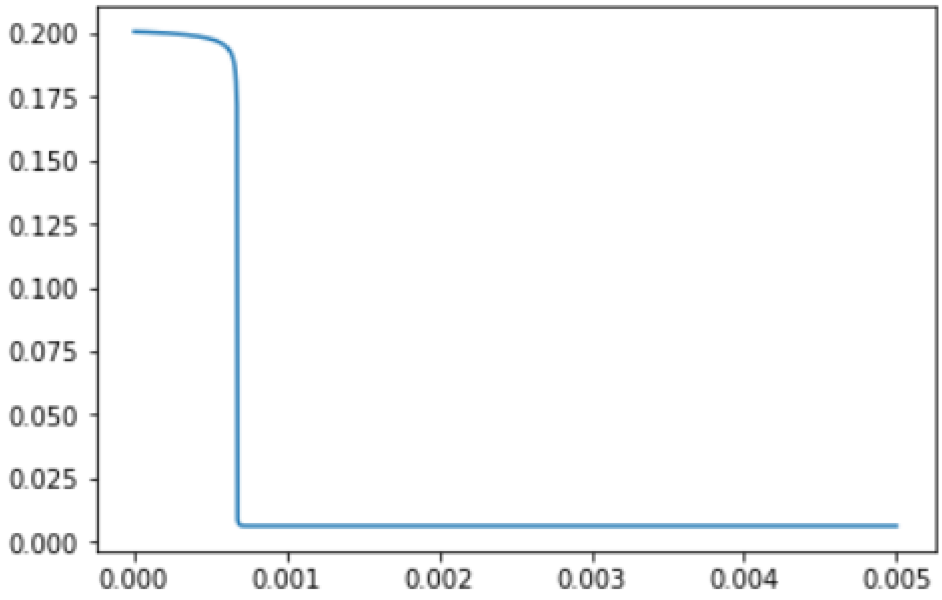
4.2. Incomplete combustion case



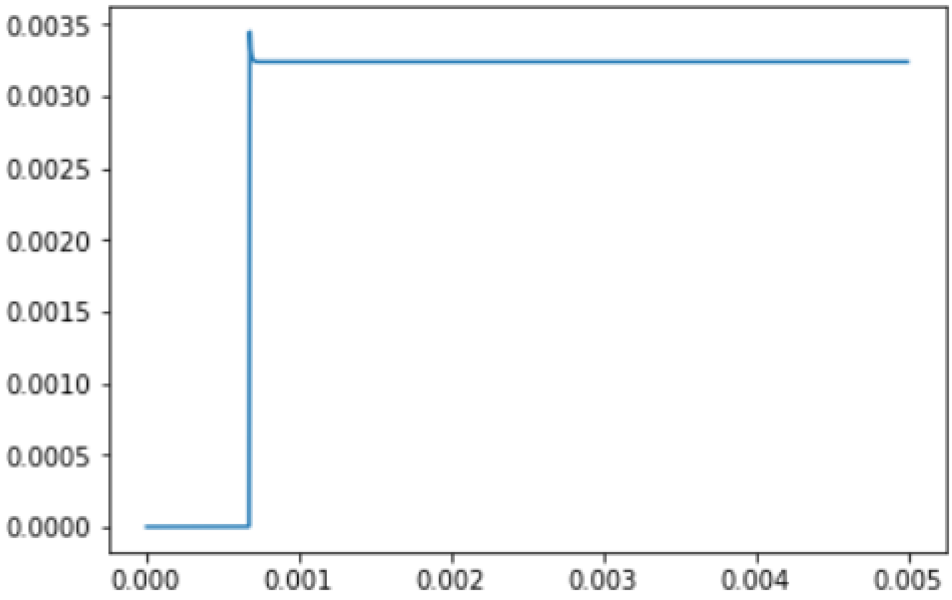
4.2.1. Temperature vs time of simulation for incomplete combustion case



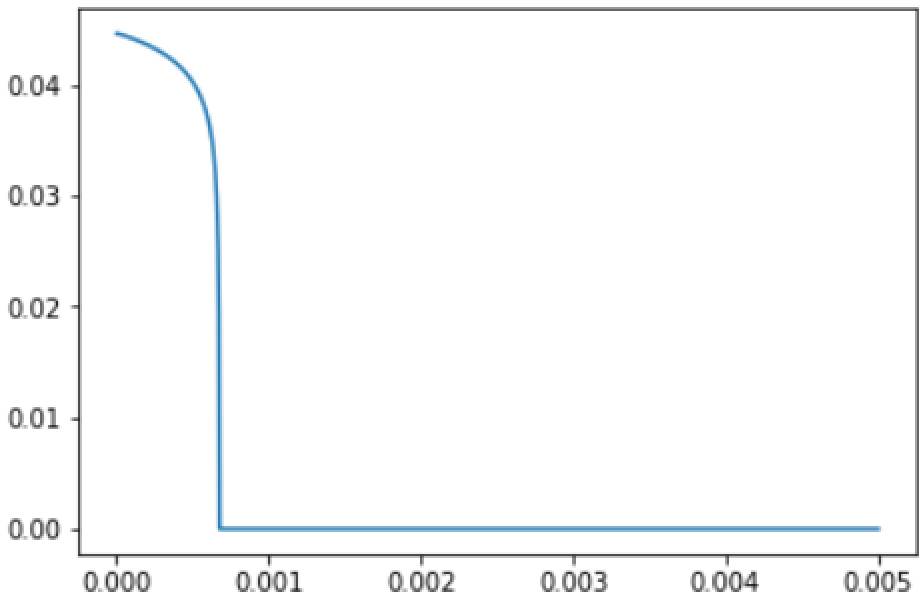
4.2.2. Pressure vs time of simulation for incomplete combustion case



4.2.3. Oxygen content vs time of simulation for incomplete combustion case



4.2.4. Hydrogen content vs time of simulation for incomplete combustion case



4.2.5. Propane content vs time of simulation for incomplete combustion case

5. Conclusions

When mixture of propane and air are together in temperature 1200K (around 900°C) and pressure is 3MPa it takes around 0,001s for it to blow up. Pressure jumps rapidly to value of 8-9 MPa, also temperature to around 3100K, which is similar to reality and what happens in 4-stroke internal combustion engine [1].
Temperature:
Incomplete combustion creates higher values of temperature 3154,22K- vs 3117,82 K in complete combustion (values in last calculated point - 999)
Pressure:
Also higher values of pressure in incomplete combustion - 8,58 MPa; for complete 8,35 MPa.
Plots for contents of gases:
Oxygen - it burns in time, by the end of both simulation hardly any of it is left - 0,0127 mol in complete; 0,0062 mol in incomplete.
Hydrogen - in both cases jumps of its content is visible - 0,0032 mol for incomplete; 0,0023 mol for complete.
Propane - for both simulations by the end of them propane is burned and values shown in plots are practically 0.

Basically those differences come from simple fact that for incomplete combustion ratio of propane to air is higher than in complete combustion case - so incomplete combustion will always be more dangerous to engine not only because it creates carbon monoxide - which is soot on engine elements but also because of higher temperature and pressure which leads to quicker destruction of a combustion chamber in engine.