# Combustion of hydrogen and oxygen in constant volume

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## 1 Introduction

The idea of this project was to create numerical model of combustion of hydrogen in oxygen. I used Cantera software for this purpose.

## 2 Literature

In order to create this project I gathered information mainly from Cantera tutorials which are available on Cantera website. I also used wikipedia pages to get basic view on the physical process of hydrogen combustion in oxygen.

## 3 Model characterization

In my code I used GRI-Mech 3.0 mechanism.GRI-Mech 3.0 is a widely-used reaction mechanism for natural gas combustion. It contains 53 species composed of the elements H, C, O, N, and/or Ar, and 325 reactions, most of which are reversible. GRI-Mech 3.0, like most combustion mechanisms, is designed for use at pressures where the ideal gas law holds.

### 3.1 Starting parameters

My program gives the user possibility to set the starting temperature by himself. Pressure and volume is set by default as follows: pressure is equal to one atmosphere, volume of the reactor is equal to one cubic meter. User is also asked to set number of oxygen and hydrogen moles.

### 3.2 Program function

After the starting parameters are set, program prints:

1. Time
2. Temperature
3. Pressure
4. Internal energy
5. Temperature in time plot
6. Number of H, OH and H2 moles in time plot
7. Temperature of combustion and time when it occurs

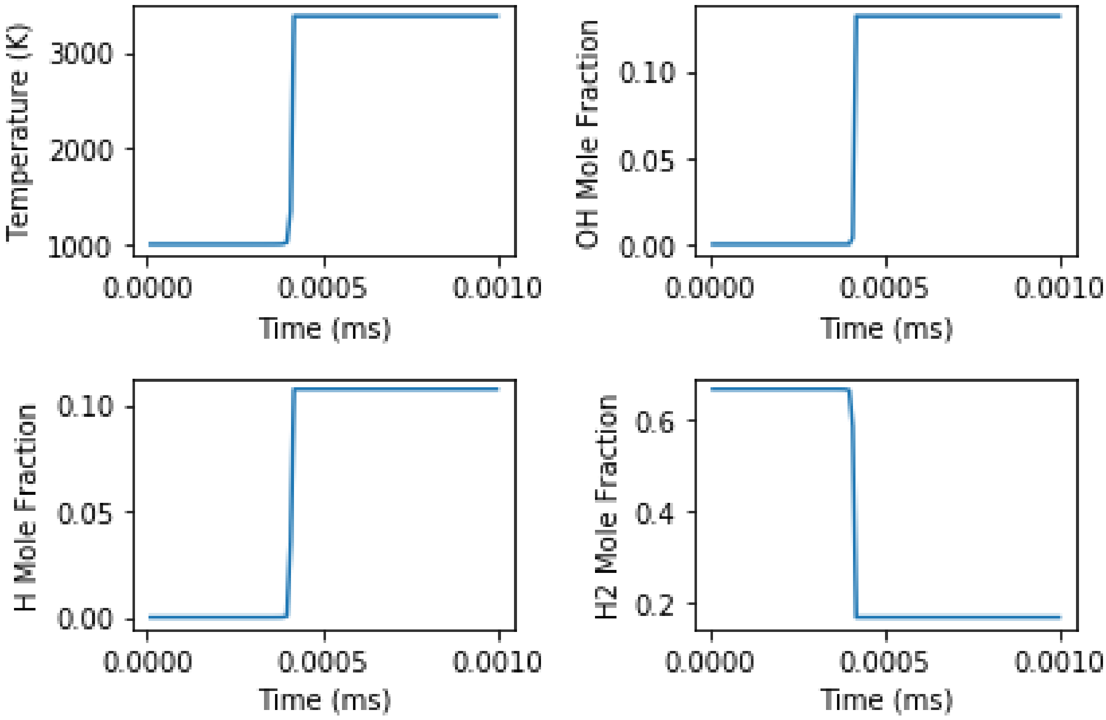
Program can be used to identify theoretical limits of combustion by setting different amounts of oxygen and hydrogen moles and analyzing the temperature and pressure.

## 4 Results

First I would like to present the results of combustion 2 moles of H2 and one mole of O2 a the temperature of 1000K: Starting parameters: Temperature: 1000.0 K Pressure: 101325.0 Pa Volume: $1.0m^3$

| t [s] | T [K] | P [Pa] | u [J/kg] |
|---|---|---|---|
| 1.000e-05 | 1000.000 | 101325.000 | 1.086203e+06 |
| 2.000e-05 | 1000.000 | 101325.000 | 1.086203e+06 |
| 3.000e-05 | 1000.000 | 101325.000 | 1.086203e+06 |
| 4.000e-05 | 1000.000 | 101325.000 | 1.086203e+06 |
| 5.000e-05 | 1000.000 | 101325.000 | 1.086203e+06 |
| 6.000e-05 | 1000.000 | 101325.000 | 1.086203e+06 |
| 7.000e-05 | 1000.000 | 101325.001 | 1.086203e+06 |
| 9.000e-05 | 1000.000 | 101325.001 | 1.086203e+06 |
| 1.000e-04 | 1000.000 | 101325.001 | 1.086203e+06 |
| 1.100e-04 | 1000.000 | 101325.001 | 1.086203e+06 |
| 1.200e-04 | 1000.000 | 101325.001 | 1.086203e+06 |
| 1.300e-04 | 1000.000 | 101325.001 | 1.086203e+06 |
| 1.400e-04 | 1000.000 | 101325.001 | 1.086203e+06 |
| 1.500e-04 | 1000.000 | 101325.002 | 1.086203e+06 |
| 1.600e-04 | 1000.000 | 101325.002 | 1.086203e+06 |
| 1.700e-04 | 1000.000 | 101325.002 | 1.086203e+06 |
| 1.800e-04 | 1000.000 | 101325.002 | 1.086203e+06 |
| 1.900e-04 | 1000.000 | 101325.002 | 1.086203e+06 |
| 2.000e-04 | 1000.000 | 101325.003 | 1.086203e+06 |
| 2.100e-04 | 1000.000 | 101325.003 | 1.086203e+06 |
| 2.200e-04 | 1000.000 | 101325.003 | 1.086203e+06 |
| 2.300e-04 | 1000.000 | 101325.003 | 1.086203e+06 |
| 2.400e-04 | 1000.000 | 101325.004 | 1.086203e+06 |
| 2.500e-04 | 1000.000 | 101325.004 | 1.086203e+06 |
| 2.600e-04 | 1000.000 | 101325.006 | 1.086203e+06 |
| 2.700e-04 | 1000.000 | 101325.018 | 1.086203e+06 |
| 2.800e-04 | 1000.001 | 101325.049 | 1.086203e+06 |
| 2.900e-04 | 1000.001 | 101325.120 | 1.086203e+06 |
| 3.000e-04 | 1000.003 | 101325.269 | 1.086203e+06 |
| 3.100e-04 | 1000.006 | 101325.578 | 1.086203e+06 |
| 3.200e-04 | 1000.013 | 101326.215 | 1.086203e+06 |
| 3.300e-04 | 1000.028 | 101327.523 | 1.086203e+06 |
| 3.400e-04 | 1000.057 | 101330.232 | 1.086203e+06 |
| 3.500e-04 | 1000.120 | 101335.953 | 1.086203e+06 |
| 3.600e-04 | 1000.256 | 101348.522 | 1.086203e+06 |
| 3.700e-04 | 1000.580 | 101378.439 | 1.086203e+06 |
| 3.800e-04 | 1001.466 | 101461.410 | 1.086203e+06 |
| 3.900e-04 | 1004.650 | 101763.815 | 1.086203e+06 |
| 4.000e-04 | 1021.651 | 103398.494 | 1.086203e+06 |
| 4.100e-04 | 1345.664 | 134203.177 | 1.086203e+06 |
| 4.200e-04 | 3378.088 | 293764.658 | 1.086203e+06 |
| 4.300e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 4.400e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 4.500e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 4.600e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 4.700e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 4.800e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 4.900e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 5.000e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 5.100e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 5.200e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 5.300e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 5.400e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 5.500e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 5.600e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 5.700e-04 | 3378.095 | 293765.121 | 1.086203e+06 |

| t [s] | T [K] | P [Pa] | u [J/kg] |
|---|---|---|---|
| 5.800e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 5.900e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 6.000e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 6.100e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 6.200e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 6.300e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 6.400e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 6.500e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 6.600e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 6.700e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 6.800e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 6.900e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 7.000e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 7.100e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 7.200e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 7.300e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 7.400e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 7.500e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 7.600e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 7.700e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 7.800e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 7.900e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 8.000e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 8.100e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 8.200e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 8.300e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 8.400e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 8.500e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 8.600e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 8.700e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 8.800e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 8.900e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 9.000e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 9.100e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 9.200e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 9.300e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 9.400e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 9.500e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 9.600e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 9.700e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 9.800e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 9.900e-04 | 3378.095 | 293765.121 | 1.086203e+06 |
| 1.000e-03 | 3378.095 | 293765.121 | 1.086203e+06 |

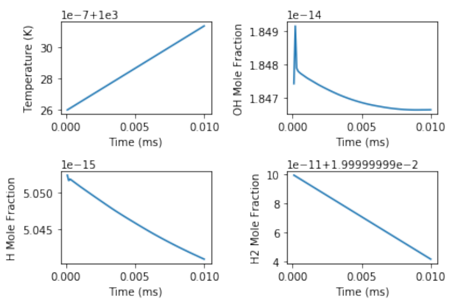



### 4.1 Combustion temperature and time of occurrence

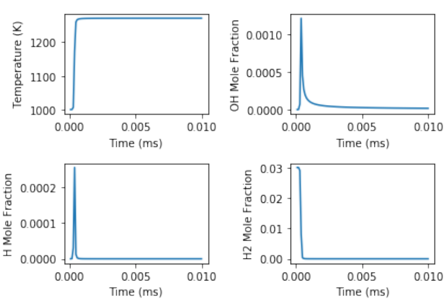
Combustion temperature and time of combustion occurrence is given when a rapid increase in temperature and pressure occurs. In this example: Combustion temperature 1345.664 K : Time of combustion occurrence: 4.100e-04 s .

## 5 Flammability limits

Lets assume that we would like to know the flammability limits for the mixture of hydrogen and oxygen with the starting temperature of 1000 K, because flammability limits are dependent of temperature. In order to achieve that we can start with the mixture composition of 1 percent hydrogen 99 percent oxygen and then increase amount of hydrogen moles by 1 percent and observe if the combustion will occur. This way we can approximately get to know the lower flammability limit.




(a) 2 percent of hydrogen

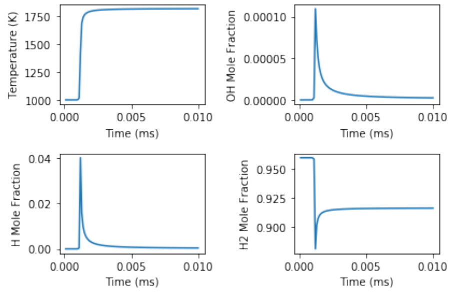



(b) 3 percent of hydrogen

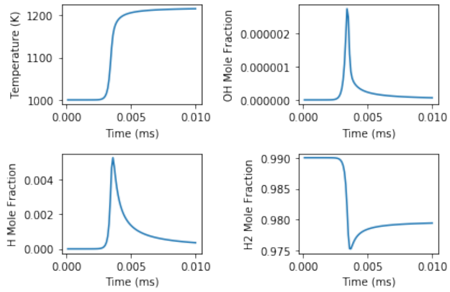
Figure 1: a) combustion does not occur b) combustion occurs

We can assume that lower flammability limit for hydrogen and oxygen is between 2 and 3 percent. In order to increase precision of calculations we can start from 2 percent and increase amount of hydrogen by smaller step, for example 0.1.

We do the same thing with higher flammability limit. We know from other sources that for mixture of hydrogen and oxygen in temperature of 293 K the HFL is equal to 96 percent of hydrogen. As I mentioned before flammability limits are dependent on temperature, as the temperature rises so does the HFL.




(a) 96 percent of hydrogen




(b) 99 percent of hydrogen

When trying to calculate the HFL we encounter a problem with this method. When increasing the percentage of hydrogen in the mixture, increase of the temperature becomes more and more subtle, and the ending temperature is lower, but the increase is still visible on plots. We cannot use this method to calculate the HFL.