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 in 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 programmes gives the user 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 Programme fuction

After the starting parameteres are set, programme 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 occures

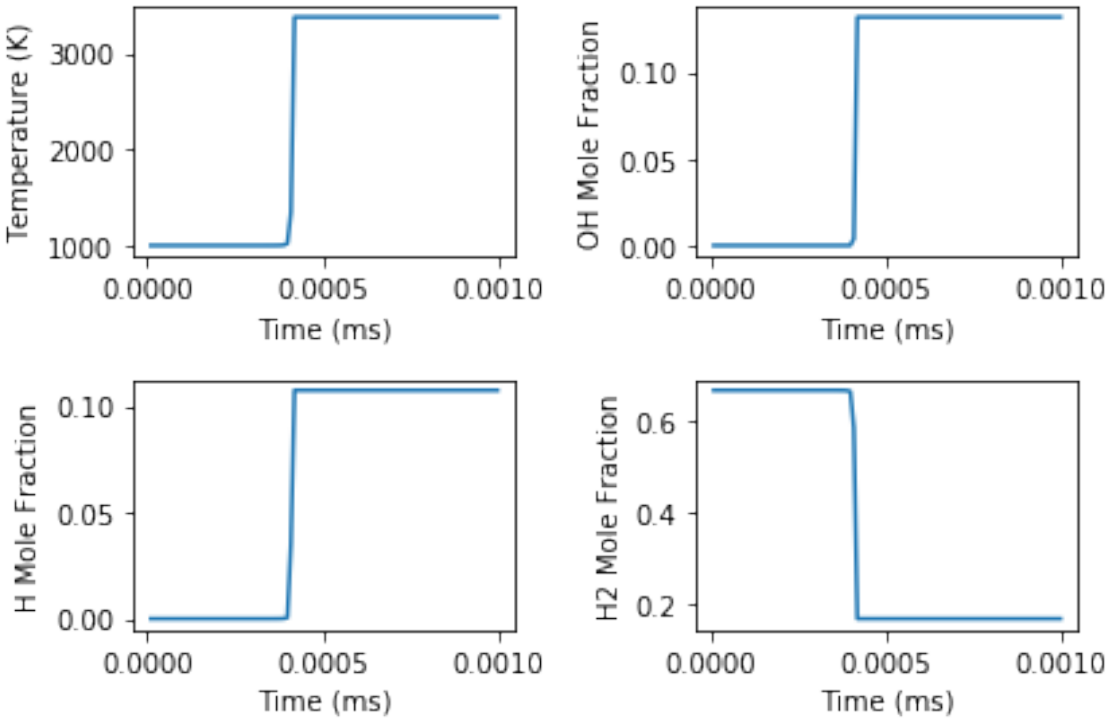
Programme can be used to identify theoretical limits of combustion by setting different amounts of oxygen and hydrogen moles and analysing the temperature and pressure.

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 ocurance

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

5 Combustion limits