Cantera Project
Laminar flame propagation speed

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1 Introduction

The main purpose of this project is to calculate laminar flame propagation speed and to check how different initial conditions of a gas influences the results. As fuel there will be used a mixture of hydrogen and air in proportions shown below. When burnt with clear oxygen, hydrogen is a "zero-emission" fuel, which means that there will be no waste products after the combustion. However, while burning in atmospheric air ,hydrogen combustion may yield small amounts of nitrogen oxides. This kind of fuel is used in many cases such as passenger cars, fuel cell buses and even in spacecraft.

2 Literature

Literature, which was used here was:

-Cantera Tutorial from offical Cantera website;

-Laminar flame speeds and ignition delay times of hydrogen-air mixtures at elevated temperatures and pressures.

3 Flame propagation speed

Laminar flame speed (SL) is the propagation velocity of a laminar flame front into the unburned premixed gas. It depends on the fuel type, air-fuel ratio, temperature and pressure. It can be calculated with good approximation by kinetic mechanisms for various fuels (such as GRI3.0 chemical reaction mechanism). The laminar flame speed is maximal near stoichiometric conditions for hydrocarbon fuels: CH4 shows maximal reactivity (fastest burning velocity) near to stoichiometric condition. For CO, and even more pronounced for H2, the maximum is shifted into the fuel rich region: maximum at stoichiometric air fuel ratio of 0.6–0.8.

4 Description of the project

In this project it was said that the gas should be a mixture of hydrogen and air. The fractions of each component was decided to be constant for every gas in this project and they were:

H2 = 0.7

Air = 1 (=> O2 = 1, N2 = 3.76)

To check the differences between different initial conditions there are three gases with the same reactants but with different temperatures and pressures. The chemical kinetic model utilized in the study includes GRIMech3.0. There are 325 elementary chemical reactions and associated rate coefficient expressions and thermochemical parameters for the 53 species in GRIMech3.0. It includes the detailed combustion reaction mechanism for hydrogen.

The first gas (gas1) has tempterature T = 300 K and pressure p = 1 atm.

The second gas (gas2) has tempterature T = 300 K and pressure p = 1.5 atm.

The third gas (gas3) has tempterature T = 400 K and pressure p = 1 atm.

When gases are defined, the program initialises flames based on them. By doing so, we get three different flames with conditions coming from gases.

5 Solution

With the flames defined, program can solve them using Cantera (which is a software tool for Python) and show results afterwards.

In this project it was decided, that the best way to examine differences between flames is making three plots of flame propagation speed for different flames on the same graph. It was possible thanks to the matplotlib library, which was imported and the beginnig.

Besides that, program will show exact numerical results on screen, so the values can be checked not only from a graph but from an array as well.

Below there is an array showing exact results from calculations for the first flame (T= 300K, p = 1 atm):

```
      Pressure:   1.013e+05 Pa

-------------------------------
          z           u
-------------------------------
          0      0.0494
      0.006     0.05191
      0.009     0.06334
     0.0105     0.08594
    0.01125      0.1099
    0.01162      0.1272
      0.012      0.1487
    0.01219      0.1604
    0.01238      0.1711
    0.01256      0.1793
    0.01275      0.1847
    0.01294      0.1879
    0.01313      0.1899
    0.01331       0.191
     0.0135      0.1917
    0.01387      0.1923
    0.01425      0.1926
      0.015      0.1928
    0.01575      0.1929
     0.0165      0.1929
      0.018       0.193
      0.024       0.193
       0.03       0.193
```

Figure 1: Numerical results for the first flame

6 Summary

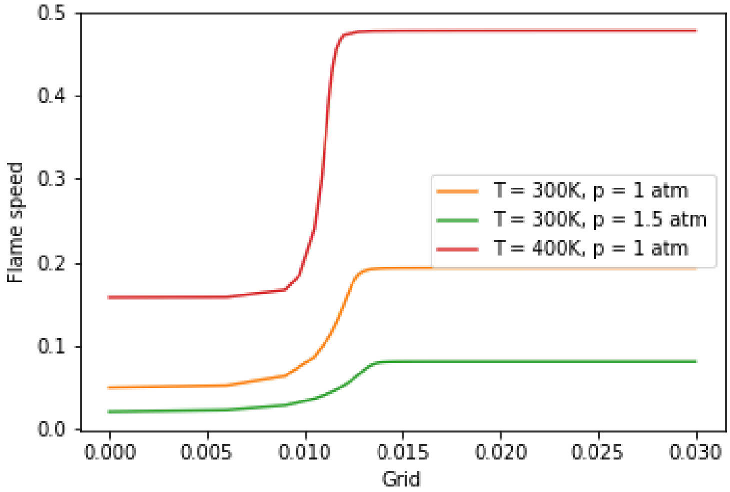

Figure 2: Flame propagation speed

As one can see, the flame propagation speed is not so high at first, but after some time it speeds up very quickly to its highest value. Moreover, for higher temperatures flame propagation is faster than for lower temperatures, however, higher pressure makes flame move slower.