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COMPUTATIONAL METHODS IN COMBUSTION

Analysis of Methane combustion in constant volume

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Contents

1 Introduction

The main goal was to investigate the parameters of methane(CH_4) during combustion in constant volume.From experimental data we know that explosion of methane-air mixture is possible within methane concentration between 4.4 to 17 percent. Concentration expressed in equivalence ratios gives us range from about 0.4 to 1.9.[1] Depending on initial conditions such as initial pressure and temperature we will get different final temperatures and pressures. To enable such an analysis, the "cantera" library was used.[2]

1.1 Chemical equation

$$CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 2 \cdot 3.76N_2 \tag{1}$$

It is stoichiometric equation of methane-air mixture. For different equivalence ratio we will get different chemical equations.

$$\varphi = \frac{(F/A)}{(F/A)_{stoich}} \tag{2}$$

1.2 Initial parameters

Range of initial pressure and initial temperature

Limits	min	max
Pressure [atm]	0.1	6
Temperature [K]	400	2000

Table 1: Initial Values

Initial concentrations

$\varphi_1 = 0.5[-]$
$\varphi_2 = 0.8[-]$
$\varphi_3 = 1[-]$
$\varphi_4 = 1.5[-]$

2 Modeling

Using "Cantera" library (implemented in python) gas model was prepared. "Numpy" library was used for numerical calculations of necessary chemical and thermodynamical equations.

```
 gri30:

       temperature   300 K
          pressure   12733 Pa
           density   0.14106 kg/m^3
  mean mol. weight   27.633 kg/kmol
   phase of matter   gas

                          1 kg             1 kmol
                     ---------------   ---------------
          enthalpy       -2.5459e+05       -7.0351e+06  J
   internal energy       -3.4485e+05       -9.5295e+06  J
           entropy            7871.8        2.1752e+05  J/K
    Gibbs function       -2.6161e+06       -7.2293e+07  J
 heat capacity c_p            1077.3             29770  J/K
 heat capacity c_v            776.45             21456  J/K

                      mass frac. Y      mole frac. X     chem. pot. / RT
                     ---------------   ---------------   ---------------
                O2           0.22014           0.19011           -28.408
               CH4          0.055187          0.095057            -56.75
                N2           0.72467           0.71483           -25.443
     [   +50 minor]                0                 0
```

Figure 1: gas properties after setting correct mixture of air-methane

Such modified gas micture was incremented into gas equiliribium with option "constant volume". In cantera we can set it using shortcut "SV".

3 Tests and results

3.1 Final temperature as a function of initial temperature at fixed pressure

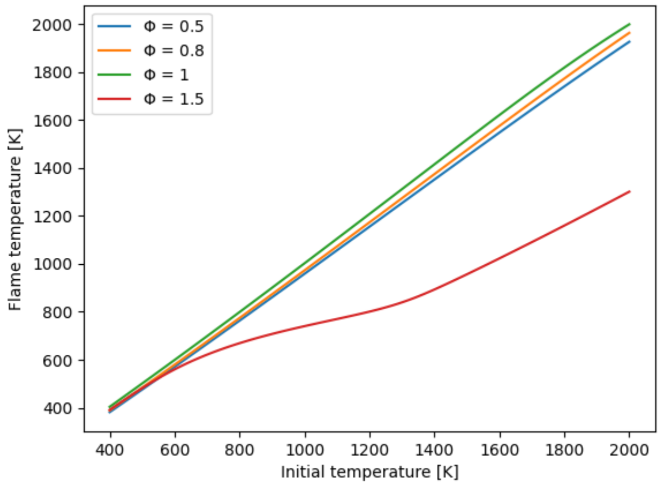

Figure 2: constant pressure= 101325 [Pa]

3.2 Final temperature as a function of initial pressure at fixed temperature

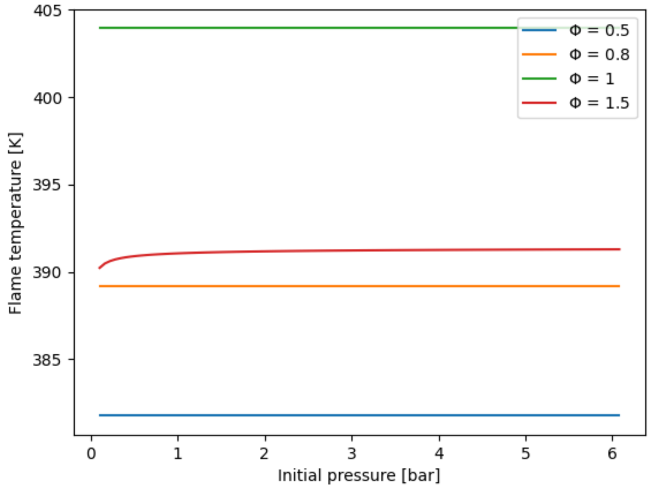

Figure 3: constatnt temperature = 400 [K]

3.3 Final pressure as a function of initial temperature at fixed pressure

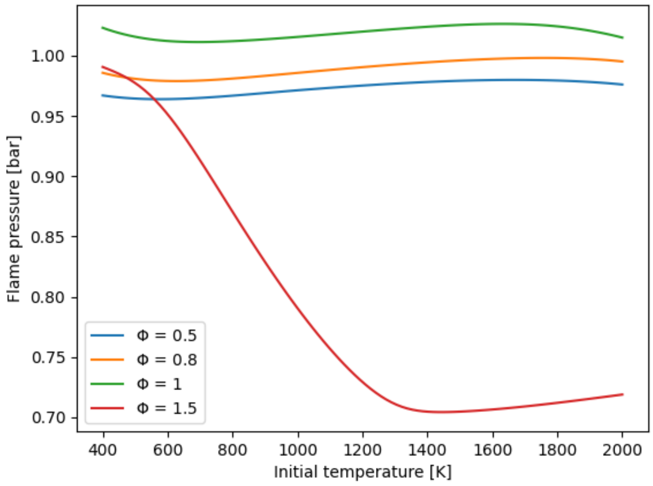

Figure 4: constant pressure= 101325 [Pa]

3.4 Final pressure as a function of initial pressure at fixed temperature

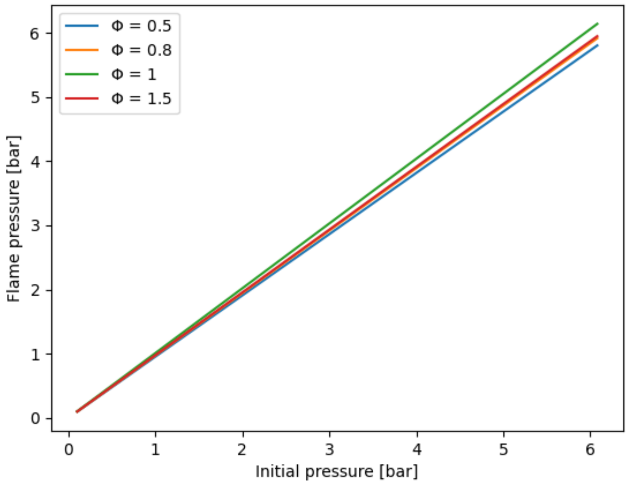

Figure 5: constatnt temperature = 400 [K]

3.5 3D pressure plots for different initial conditions

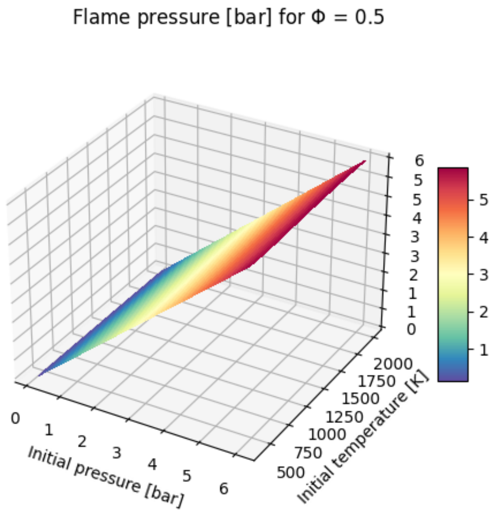

Figure 6: Final pressure for $\varphi_1 = 0.5$

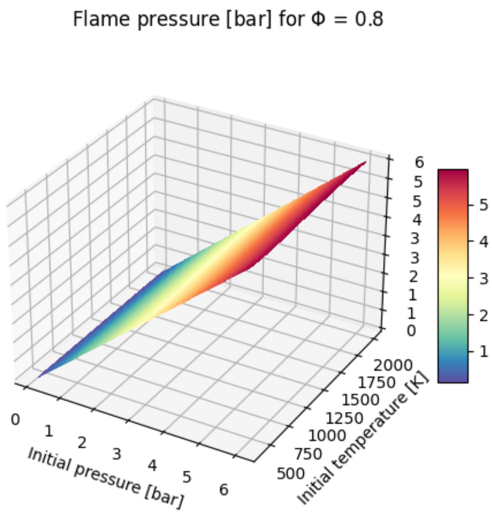

Figure 7: Final pressure for $\varphi_2 = 0.8$

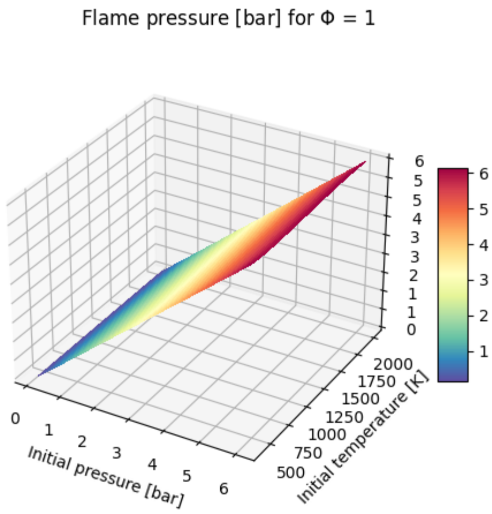

Figure 8: Final pressure for $\varphi_3 = 1$

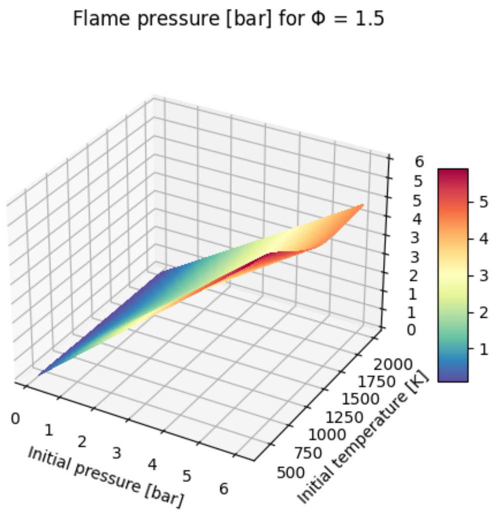

Figure 9: Final pressure for $\varphi_4 = 1.5$

3.6 3D temperature plots for different initial conditions

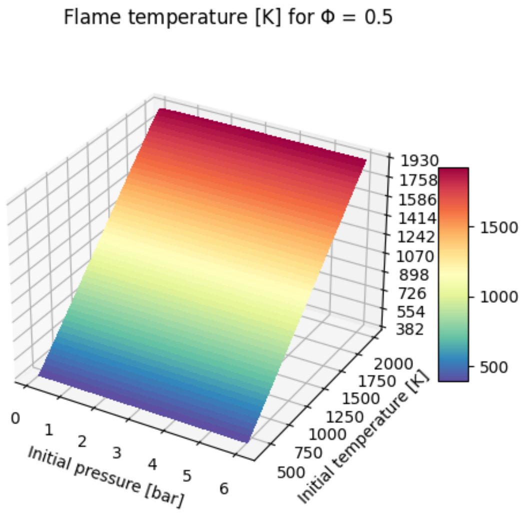

Figure 10: Final temperature for $\varphi_1 = 0.5$

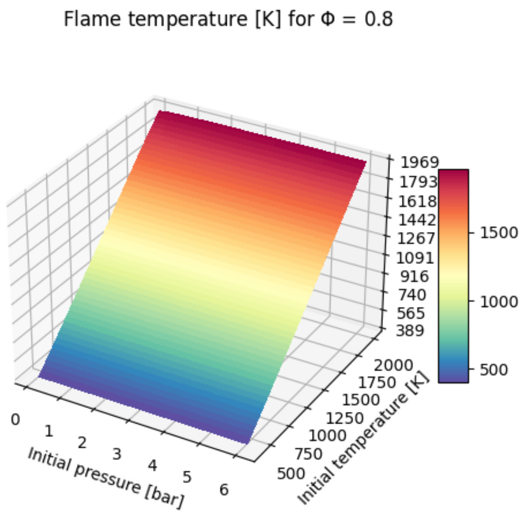

Figure 11: Final temperature for $\varphi_2 = 0.8$

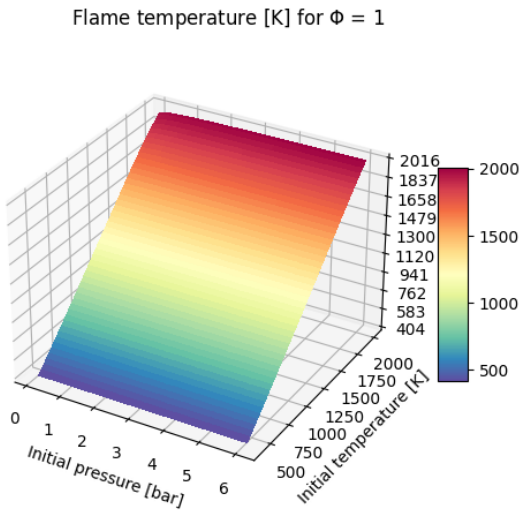

Figure 12: Final temperature for $\varphi_3 = 1$

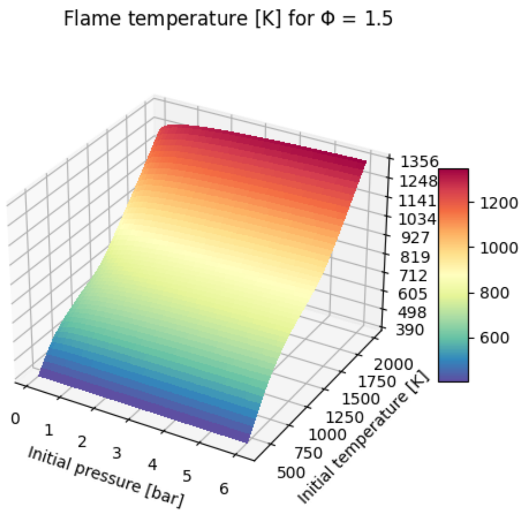

Figure 13: Final temperature for $\varphi_4 = 1.5$

4 Summary and Conclusions

Flame temperature with constant volume depends almost linearly on initial temperature [Figure 2]. One exception occurs in a plot where equivalence ratio equals 1.5. This may be because it is close to the flammability burning limit.

[Figure 3] shows that final temperature is almost independent on initial pressures. In this case final temperature only depends on different equivalence ratios. It can be noticed that for stoichiometry the final temperature is the highiest.

Another conclusion is that final pressure is almost independent of the initial temperature(when initial pressure is fixed) during the process. Once again, there is one exception. When equivalence ratio is above stoichiometric we can see a significiant drop of flame pressure as the initial temperature increases [Figure 4] for different initial pressures, the final pressures satisfy an almost linear relationship which we can see on [Figure 5].

To sum up, we can say that stoichiometric concentration of methane in air gives us the greatests flame temperatures and pressures in every situation.

More accurate maps of pressures or temperatures versus initial pressures and temperatures are shown on the 3d charts. However, they are more illustrative than readable.

References

[1] *https://en.wikipedia.org/wiki/Flammability_limit*.

[2] *https://cantera.org/documentation/*.

[3] *materiały dostarczone przez prowadzącego na kanale teams*.