Metody Komputerowe w Spalaniu

Laminar flame combustion - 1D approach

Wydział Mechaniczny Energetyki i Lotnictwa

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1 Introduction

The aim of the project is to analyze laminar flame for sensitivity of ignition velocity and its maximum temperature depending on stoichiometry of the mixture air - fuel. Based on end results it is possible to check if the area where there is just enough oxygen to burn all the fuel is also the one with most "extreme" conditions. It allows us to tell how this kind of simulation relates to the real problem. Additionally the user can observe how fractions of the mixture change throughout the calculations for different amounts of fuel.

2 Main assumptions

It was decided to use one dimensional model. The problem is relatively simple and repetitive therefore there is no need to complicate it and expand computation time. Process is shown on the illustration below:

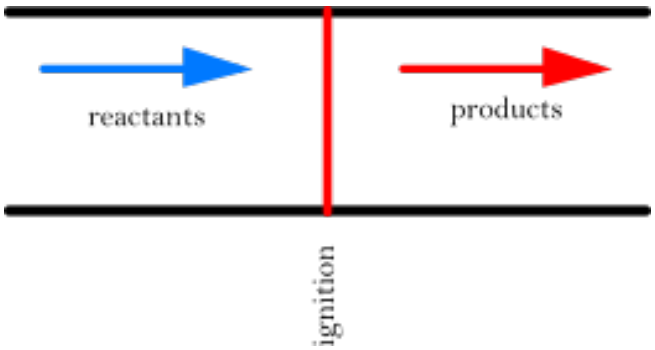


Figure 1: Temperature as function of mixture species mole fractions

Computations are executed for parameters listed below:

- $p = 101325$ Pa - pressure before the ignition point
- $T = 300$ K - temperature before the ignition point
- $d = 0.1$ m - domain width

3 Solution design and operation

As it was stated in previous paragraph, solution is simplified to the 1D case. *Flame* solver is the one that meets all the needs just perfectly. Its complexity, already built in *cantera*, makes the rest of the code and all accuracy settings simple and accessible, yet reliable. Firstly code asks the user to put pressure and temperature values. These are start parameters of the mixture, that will be used for all the calculations. Mixture itself is declared in code as ideal gas and the fuel used in the project is ethane (C_2H_6). Last parameter that needs to be given is the equivalence ratio - ratio of the actual fuel/air ratio to the stoichiometric ratio. This declaration has one significant defect - setting amount of fuel as equivalence ratio implies that fuel burns completely and certainly with minimum amount (known by *cantera*) of oxidant. It means that solution doesn't check whether equivalence is 1 for the right fraction of mixture species. It just assumes it is there. However declaration works fine for demanded results. Same declarations of parameters and solution itself are put in the *for* loop. It makes getting to the finish results much faster as there is no need to enter another equivalence ratio each time - maximum temperature of the flame and ignition velocity are saved after every iteration. They are used for the 2 final plots, making easy to compare all iterations and draw conclusions.

4 Results and conclusion

All the results are shown on plots:

- summary plots as the function of mixture stoichiometry (points on those graphs were concentrated around the area where some changes were expected)
  - flame velocity at the ignition point,
  - maximum temperature.
- plots for separated iterations as the function of y [cm] - distance along the flame:
  - temperature,
  - mole fractions of mixture species.

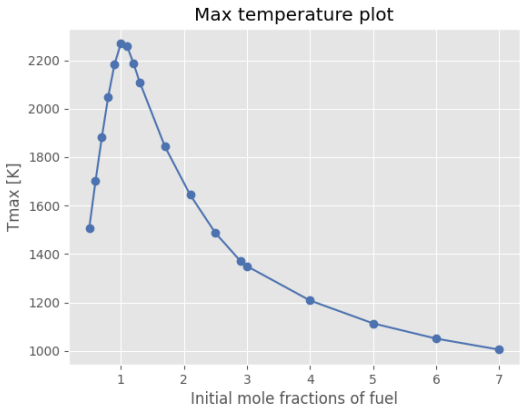


Figure 2: Temperature as function of mixture species mole fractions

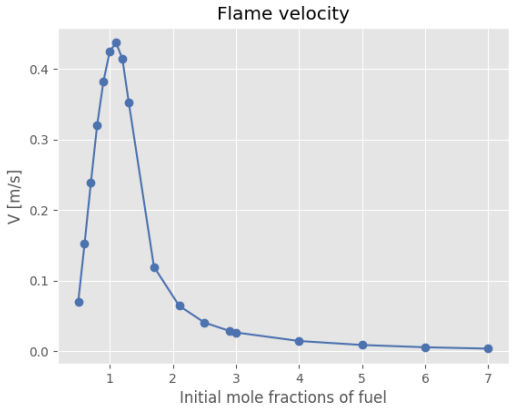
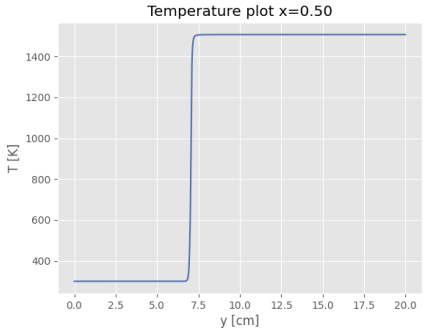
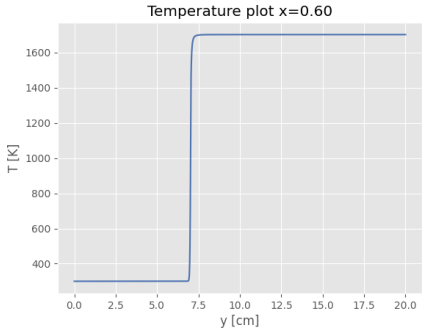


Figure 3: Velocity as function of mixture species mole fractions


Temperature plot x=0.50
T [K]
y [cm]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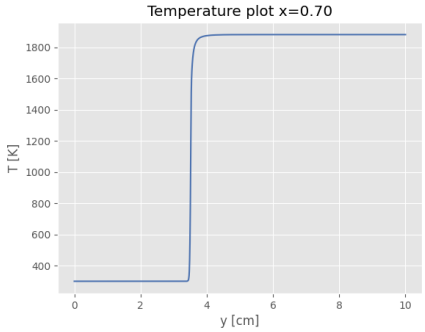
y [cm]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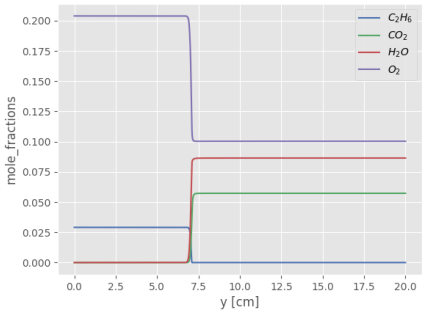
T [K]
y [cm]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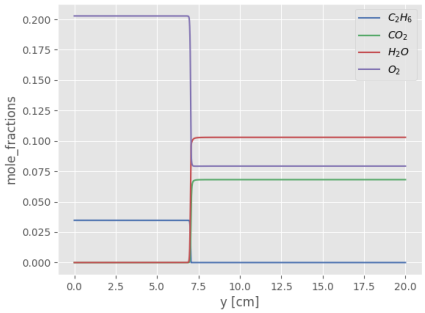
y [cm]
C_2H_6
CO_2
H_2O
O_2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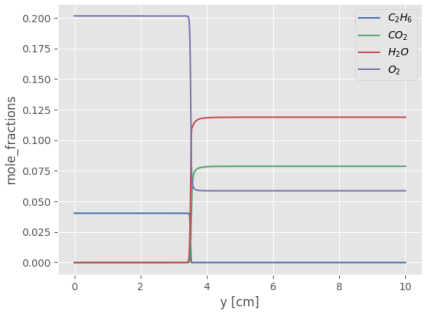
y [cm]
C_2H_6
CO_2
H_2O
O_2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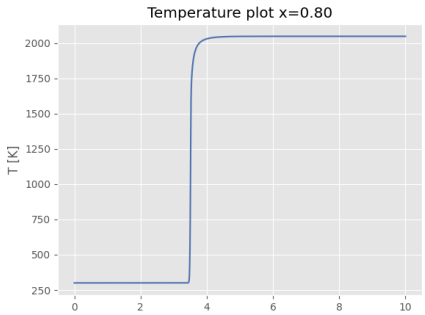
y [cm]
C_2H_6
CO_2
H_2O
O_2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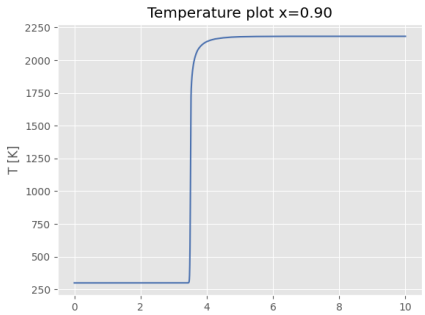
T [K]
y [cm]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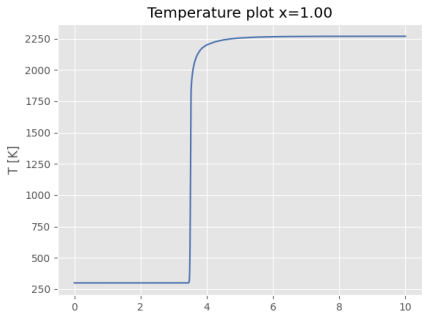
T [K]
y [cm]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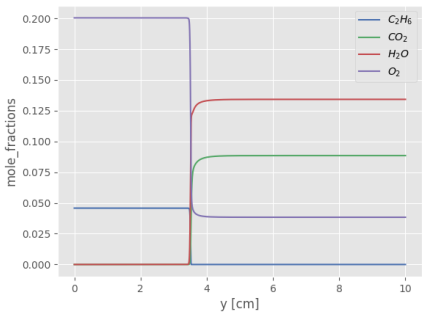
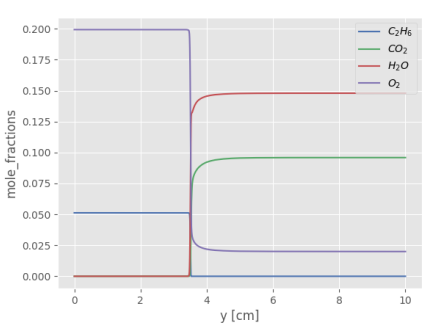
T [K]
y [cm]


mole_fractions
y [cm]
C_2H_6
CO_2
H_2O
O_2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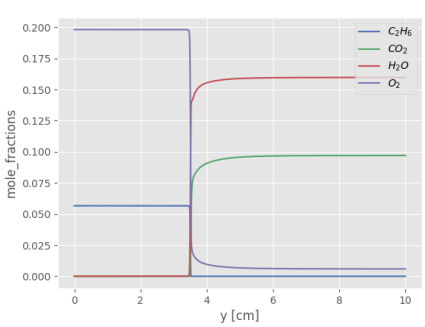
y [cm]
C_2H_6
CO_2
H_2O
O_2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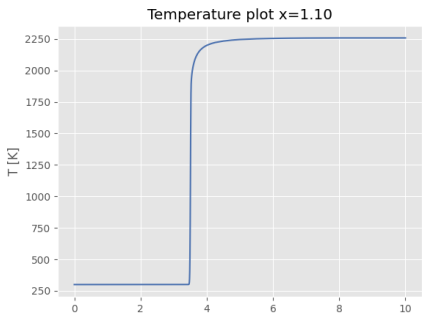
y [cm]
C_2H_6
CO_2
H_2O
O_2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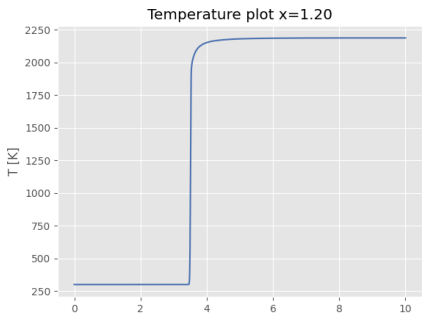
T [K]
y [cm]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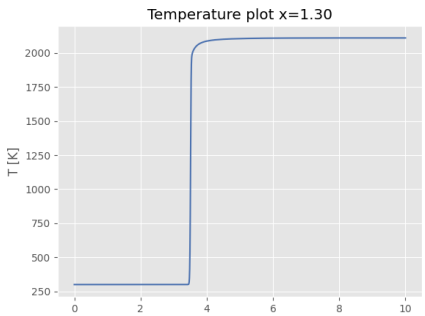
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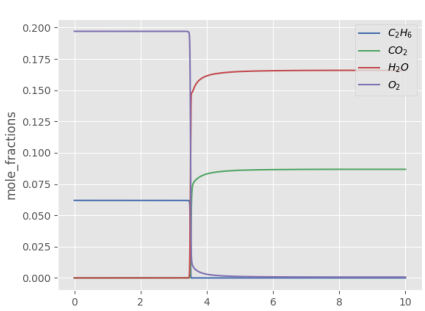
T [K]
y [cm]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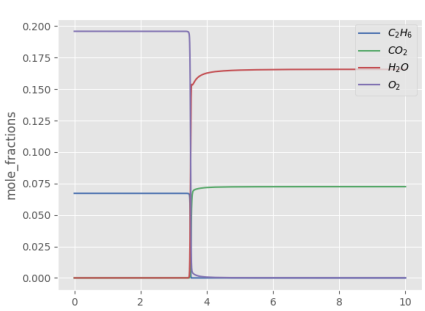
y [cm]
C_2H_6
CO_2
H_2O
O_2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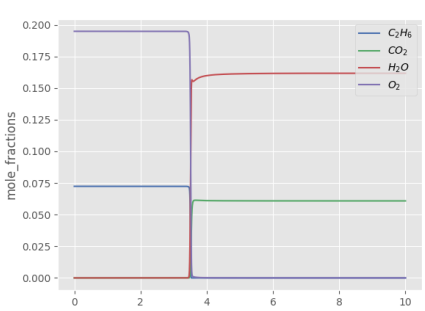
CO_2
H_2O
O_2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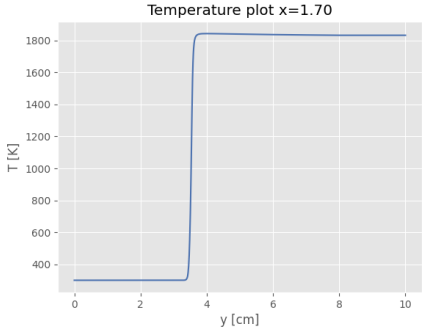
y [cm]
C_2H_6
CO_2
H_2O
O_2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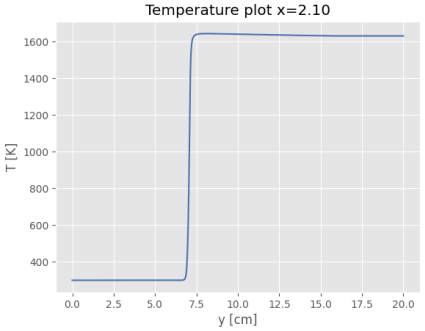
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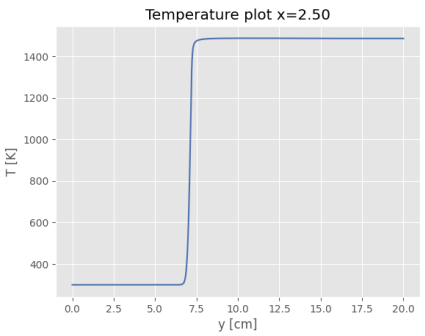
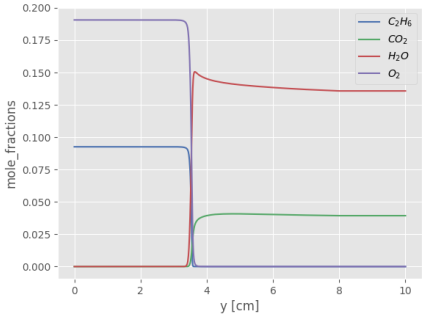
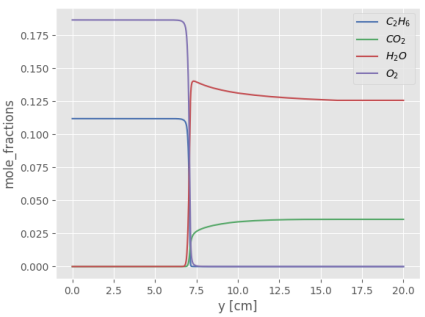

Temperature plot x=2.50
T [K]
y [cm]


C_2H_6
CO_2
H_2O
O_2
mole_fractions
y [cm]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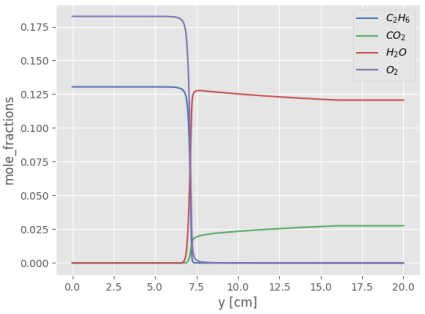
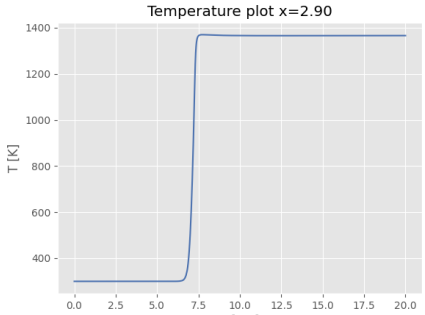
CO_2
H_2O
O_2
mole_fractions
y [cm]


C_2H_6
CO_2
H_2O
O_2
mole_fractions
y [cm]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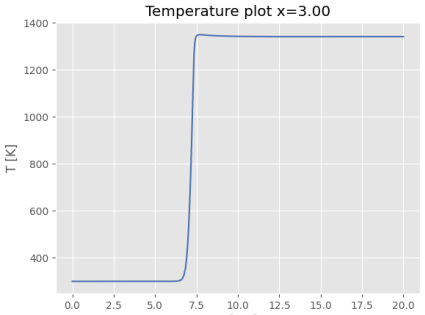
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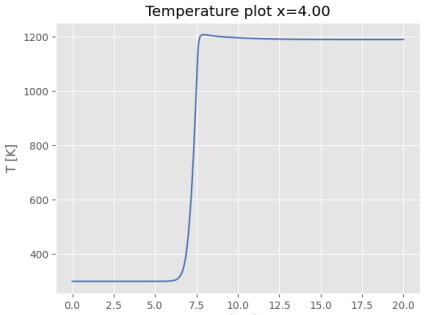
y [cm]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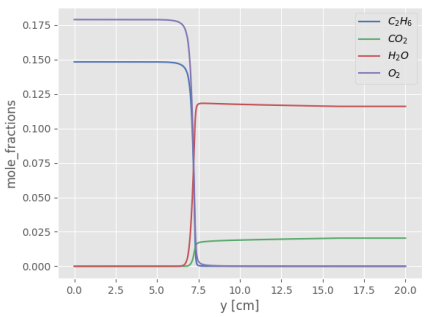
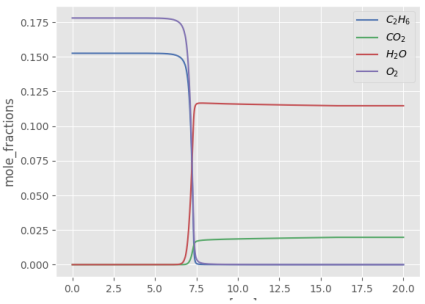
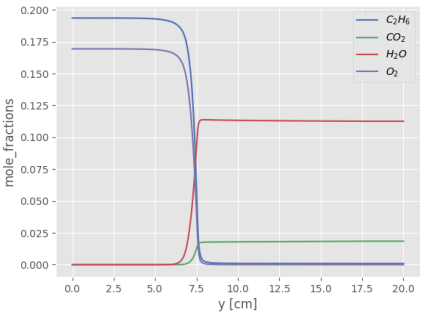
y [cm]


C_2H_6
CO_2
H_2O
O_2
mole_fractions
y [cm]


C_2H_6
CO_2
H_2O
O_2
mole_fractions
y [cm]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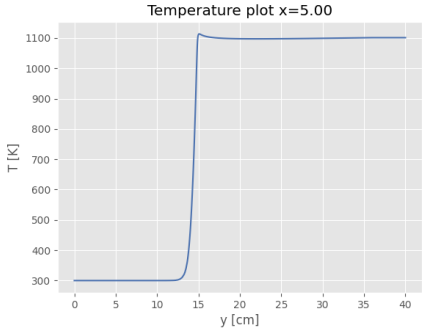
CO_2
H_2O
O_2
mole_fractions
y [cm]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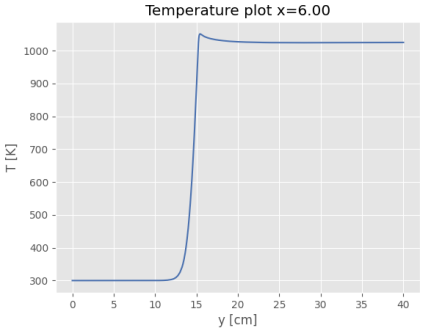
T [K]
y [cm]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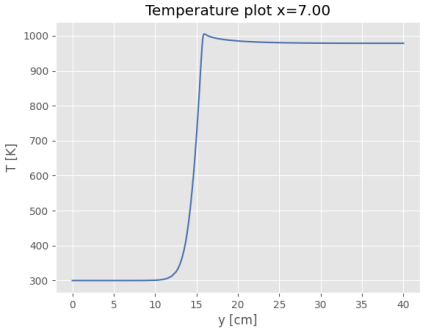
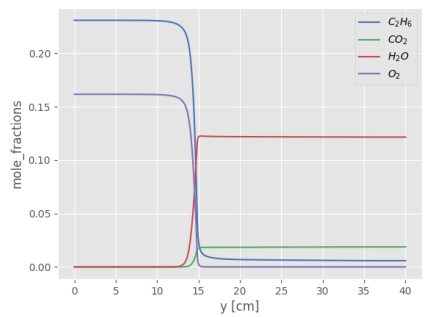
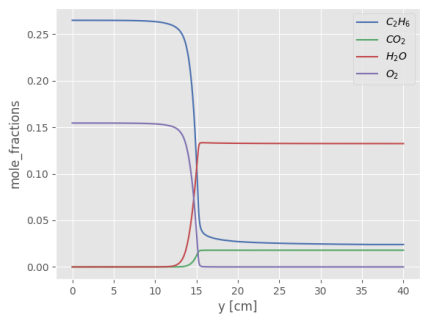
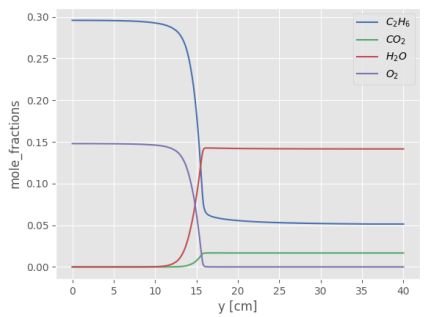
y [cm]


Temperature plot x=7.00
T [K]
y [cm]


C_2H_6
CO_2
H_2O
O_2
mole_fractions
y [cm]


C_2H_6
CO_2
H_2O
O_2
mole_fractions
y [cm]


C_2H_6
CO_2
H_2O
O_2
mole_fractions
y [cm]

As expected maximum temperature of the flame were at the point of equivalence ratio equal to 1. What is actually interesting, ignition velocity value which is the highest, is a bit above expected point (1). In real life case we would believe that temperature with higher excess air factor would decrease slightly slower than the one with too much fuel. It happens because unburnt fuel tends to cool combustion area. Received results in fact seem to match those gradient characters, however it must be emphasized that used algorithm probably doesn't include this kind of complexity. Plots of mixture species mole fractions also meet expectations - there is no enough fuel, fumes (products) amount is lower. The most surprising and unclear is character of mole fractions of water line. Around $\phi = 1.7$ plot reaches its maximum and then starts decreasing. Summing up overall quality of applied solution gives satisfying and reliable results.

5 Sources

- `https://cantera.org/examples/jupyter/flames/flame_speed_with_sensitivity_analysis.ipynb.html`
- `https://cantera.org`
- `https://numpy.org/doc/stable/user/quickstart.html`