

1-D flame speed analysis for methane and hydrogen combustion mechanism

Julia Michalec

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1 Introduction

The analysis of 1-D flame speed is the measured rate of expansion of a flame front in a combustion reaction. The flame is a small disturbance that passes along the combustion area. The analysis shows how the flame propagates. The flame propagates forward unburned gases (at any time flame occupies only small part of the combustible mixture).

2 Description of the model

The analysis starts with writing down the equation of combustion of the methane and for the next case the combustion equation for the hydrogen. For these project, we consider an equivalence ratio of 0.9 (lean mixture).

Methane: $0.9CH_4 + 2(O_2 + 3.76N_2) \rightarrow 0.9CO_2 + 1.8H_2O + 7.52N_2 + 0.2O_2$

Hydrogen: $1.8H_2 + O_2 + 3.76N_2 \rightarrow 1.8H_2O + 3.76N_2 + 0.1O_2$

The initial pressure is set to 1 atm and initial temperatures are set to 300, 325, 350, 375 and 400 K for different cases for both methane and hydrogen. The length of the domain is 0.05 m.

The Cantera solver obtains a solution for a coarse grid using the Newton-Raphson method. The solution is then monitored for gradients and curvature and subsequent grid refinement is done at the points of interest. The mechanism we use is the gri30.xml.

3 Literature

The flame speed and its temperature depends on the percentage of the elements in the mixture, the equivalence ratio and the initial conditions. The first factor affecting flammability is the mole fractions of the species in the mixture. The closer to the stoichiometric composition the better combustion conditions. If mixture is too lean or too rich it could be hard to combust it. The same applies to the equivalence ratio which corresponds to combustion under stoichiometric conditions [2]. The initial conditions are pressure and the temperature at the start of the combustion. The adiabatic temperature of the flame is the temperature that occurs when during combustion without heat loss. For methane-oxygen mixture the temperature is 2233 K and for hydrogen-oxygen mixture it is 2365 K (according to [1]).

4 Results

4.1 Methane- oxygen mixture

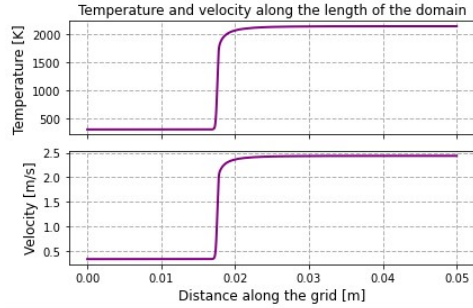


Figure 4.1: Methane- oxygen mixture combustion, temperature 300 K

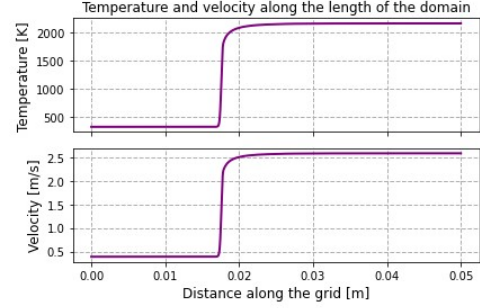


Figure 4.2: Methane- oxygen mixture combustion, temperature 325 K

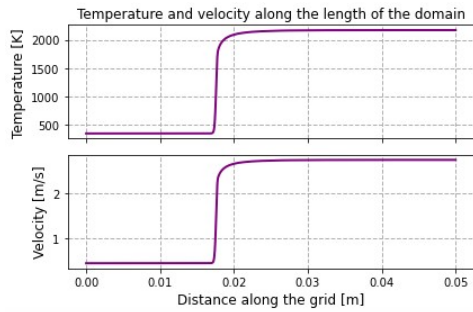


Figure 4.3: Methane- oxygen mixture combustion, temperature 350 K

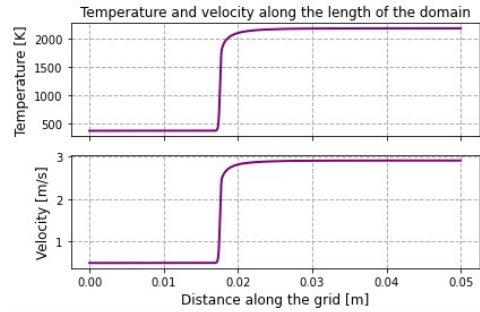


Figure 4.4: Methane- oxygen mixture combustion, temperature 375 K

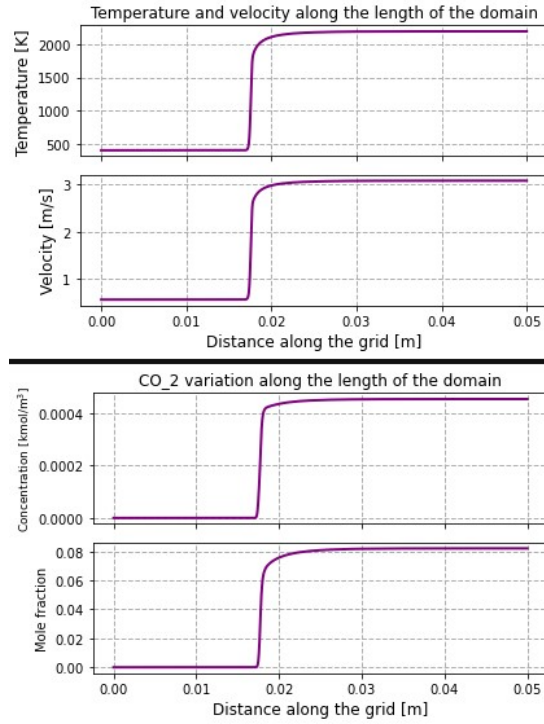


Figure 4.5: Methane- oxygen mixture combustion, temperature 400 K

The graphs clearly show that the temperature and velocity increase rapidly about 0.017m from the beginning of the domain. The temperature reaches about 2300 K. Shortly after the increase both parameters stabilize at a constant levels. The CO_2 variation along the length of the domain increases at the same point and in the same way as previously mentioned parameters.

4.2 Hydrogen- oxygen mixture

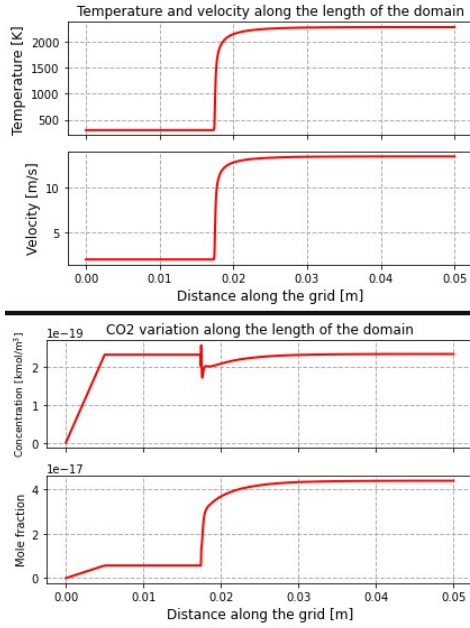


Figure 4.6: Hydrogen- oxygen mixture combustion, temperature 300 K

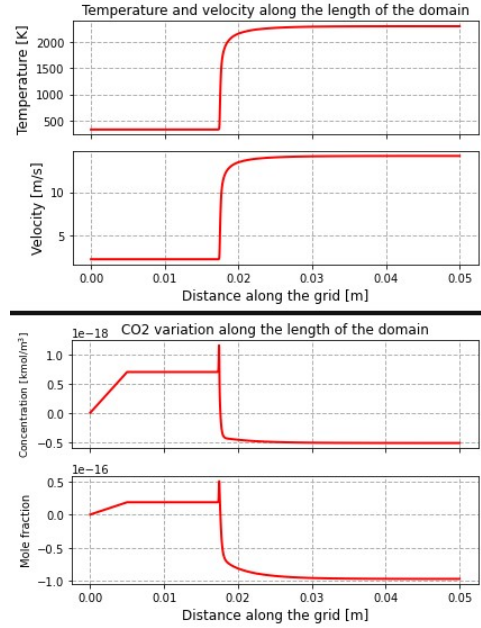


Figure 4.7: Hydrogen- oxygen mixture combustion, temperature 325 K

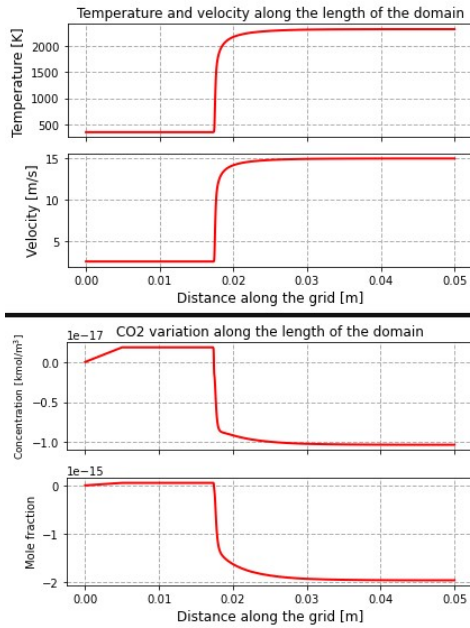


Figure 4.8: Hydrogen- oxygen mixture combustion, temperature 350 K

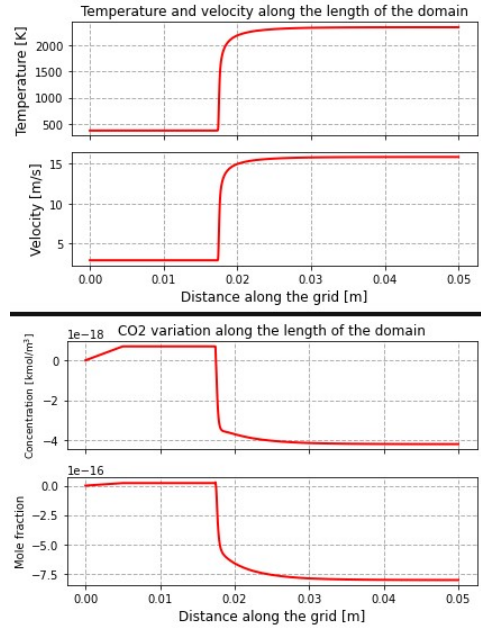


Figure 4.9: Hydrogen- oxygen mixture combustion, temperature 375 K

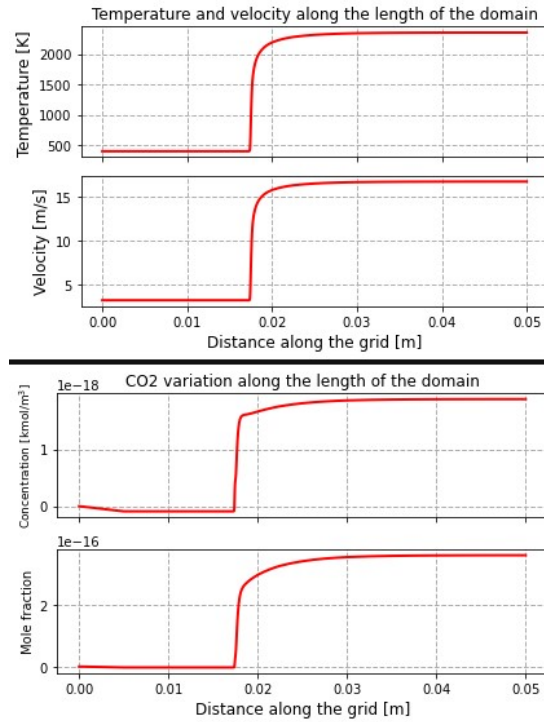


Figure 4.10: Hydrogen- oxygen mixture combustion, temperature 400 K

The charts show the temperature and flame velocity increase dramatically for all cases. The graphs of the CO_2 variation along the length of the domain have different course depending on the initial temperature. For initial temperatures 300 K and 400 K CO_2 concentration and mole fraction increase at the same point of the domains as temperature and velocity. For 325, 350 and 375 K these parameters decrease and reach negative values.

Type of mixture	Temperature [K]	Velocity $\frac{m}{s}$
CH_4 and O_2	300	0.340649
	325	0.388917
	350	0.441274
	375	0.497458
	400	0.558209
H_2 and O_2	300	2.031935
	325	2.310960
	350	2.610663
	375	2.931137
	400	3.270790

Figure 4.11: Hydrogen- oxygen mixture combustion, temperature 400 K

5 Conclusions

During analysing of the graphs above you can see that the velocity of the flame accelerate proportionally to the initial temperature. The flame speed of the hydrogen- oxygen mixture is much higher than the flame speed of methane- oxygen mixture, which agrees with the literature values and the fact that hydrogen has a higher speed of laminar combustion than methane ([1]).

When examining the temperature graphs you can see that the temperature rises more rapidly for higher initial temperature.

The same conclusion comes during analysing the CO_2 variation along the length of the domain for the methane. The graphs for the hydrogen have an unstable course which can be caused by the gri30.xlm mechanism. That mechanism has been optimized for the combustion of hydrocarbones. What is more the CO_2 variation along the length of the domain for hydrogen shows that the hydrogen combustion occurs more aggressively than the methane combustion.

6 Sources

[1] "Adiabatyczna temperatura płomienia oraz prędkość spalania laminarnego dla mieszanin CH_4/H_2 /powietrze"- W.Jerzak

[2] "Fundamental studies of premixed combustion"- Md. Z. Haq

[3] <https://skill-lync.com/projects/1-D-flame-speed-analysis-for-methane-and-hydrogen-combustion-mechanisms-using-Python-and-Cantera-27950?fbclid=IwAR1-ddZpbV-Wej6jA7ot0b2mV0GFZ-ak2cPs4xUZ3wWCBoxg5puDugznI>

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