The Temperature and Heat combustion

1. Introduce

Temperature of combustion is evaluated from the balance of subtracts and products enthalpies under constant pressure.

The heat of combustion is the energy liberated when a substance undergoes complete combustion, at constant pressure usually in an environment with excess Oxygen. The heat of combustion is used to check the performance of a fuel in a combustion system such as aircraft engins or power generation turbines. The heat of combustion is typically presented in the form of a heating value. The heating value is the amount of energy released during combustion and can be referenced as a higher or lower heating value.

The higher heating value (HHV) accounts for the heat of combustion and any energy released to bring the combustion products back their pre-combustion temperatures. By bringing the combustion products back to pre-combustion temperatures, the water component of the combustion products condenses and therefore the latent heat of vaporisation of water is incorporated in the higher heating value.

The lower heating value (LHV) assumes that the combustion products are not breaing back to pre-combustion temperatures and is therefore essentially the higher heating value minus the latent heat of vaporisation of the water product.

Coreletion

$$HHV = LHV + H_V \left(\frac{n_{H2O,out}}{n_{fuel,in}} \right)$$

where H_v is the heat of vaporization of water, $n_{H2O,out}$ is the moles of water vaporized and $n_{fuel,in}$ is the number of moles of fuel combusted.

Typically measuring of heating values is making in normal temperature 25 and pressure of 1 bar

2. Model

Temperatures – the model measures the temperatures of combustion three different fuels. The model is using a reactor with constant pressure and saving temperatures in every 0,00005 second starting from 0 to 0,005 second. The results are shown on plots were on X axis is time and on a Y axis is a temperature.

Initial conditions:

- $T_1 = 900\ [K]$ $\quad p_1 = 101325\ [Pa]$
- $T_2 = 1000\ [K]$ $\quad p_2 = 1{,}5\ [bar]$
- $T_3 = 1200\ [K]$ $\quad p_3 = 3\ [bar]$

Fuels

- Methane (CH4)
- Propane (C_3H_8)
- Hydrogen (H_2)

Heating values - the model measures the heating values of three different mixture with three different initial conditions. Model is using a enthalpy mass of substrate and products which are in cantera mechanism giri30. The result is made by substraction enthalpy mass between products and substrates. To calculate a HHV model includes also a heat of vaporisation of water.

Initial conditions:

- $T_1 = 298\ [K]$ $\quad p_1 = 101325\ [Pa]$
- $T_2 = 400\ [K]$ $\quad p_2 = 1{,}5\ [bar]$
- $T_3 = 600\ [K]$ $\quad p_3 = 3\ [bar]$

Mixtures

- Methane (CH4)

$$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$$

- Propane (C_3H_8)

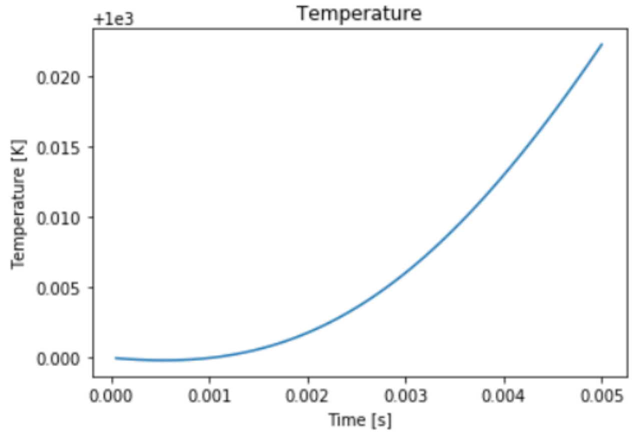
$$C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O$$

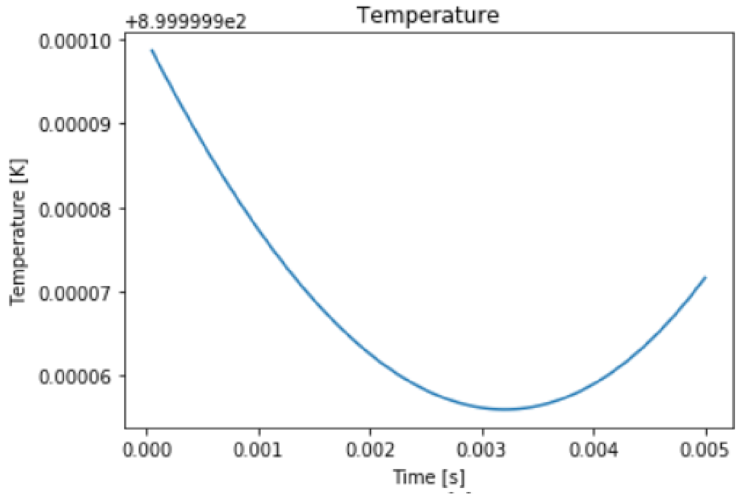
- Hydrogen (H_2)

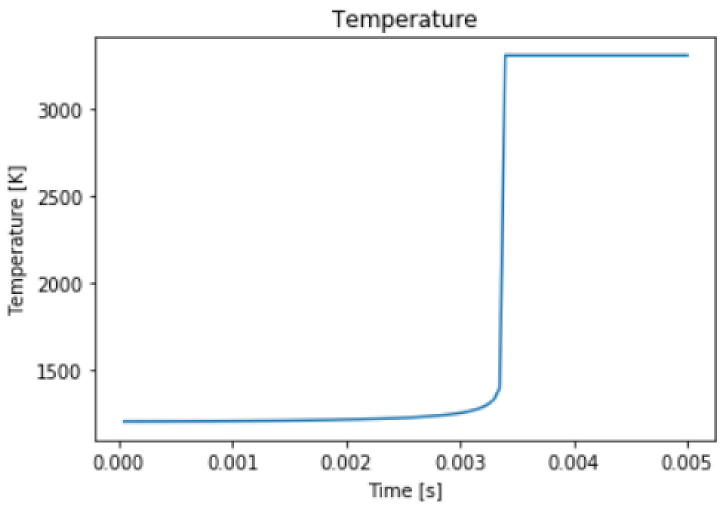
$$2H_2 + O_2 \rightarrow 2\ H_2O$$

3. Results

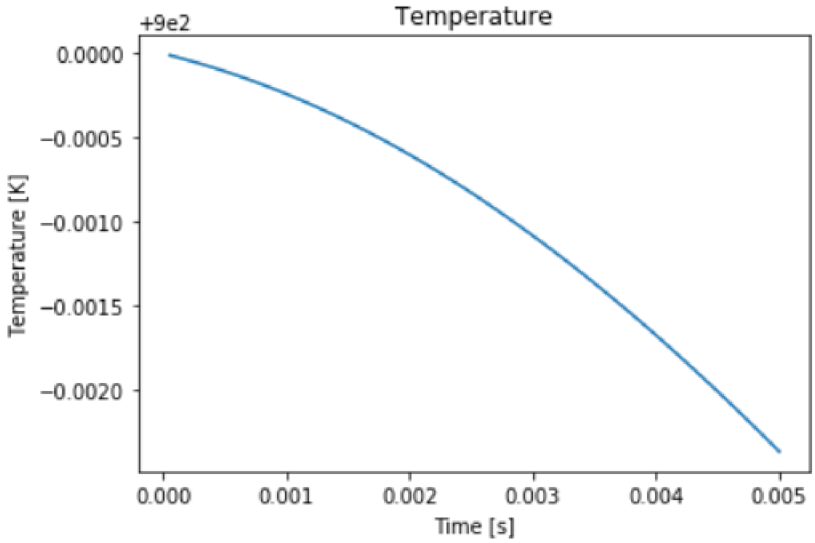
- Temperatures
  - Fuels
    - Methane (CH4)

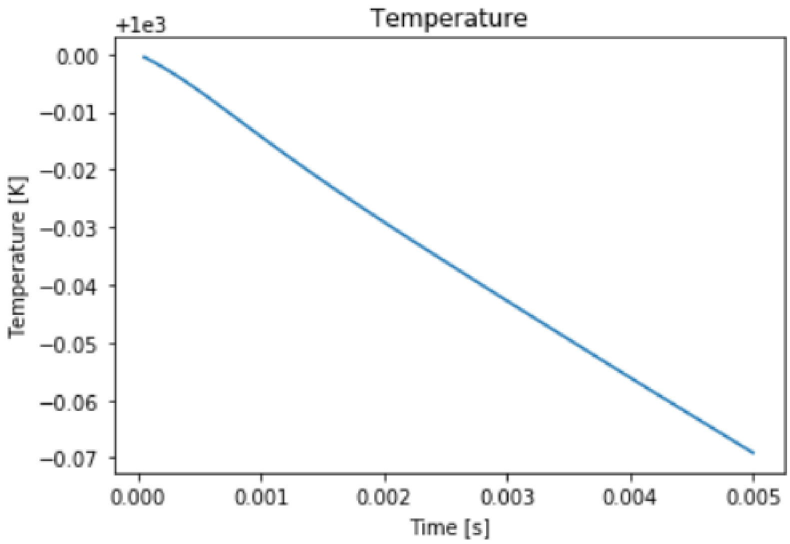


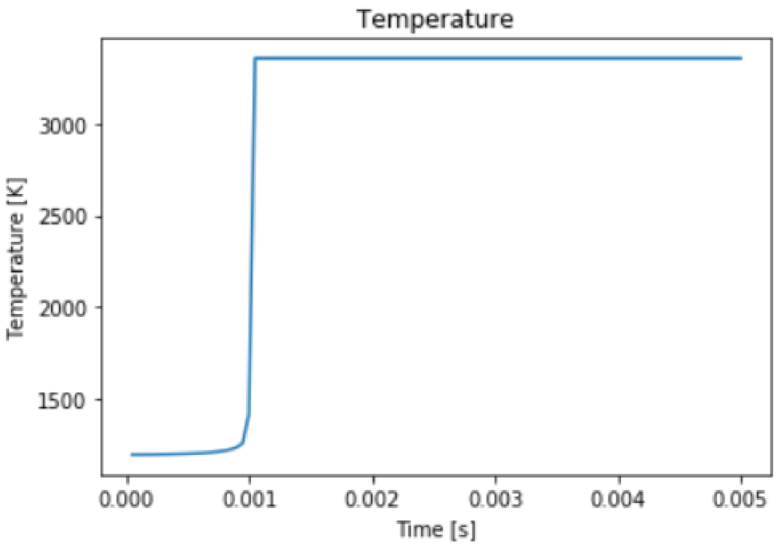




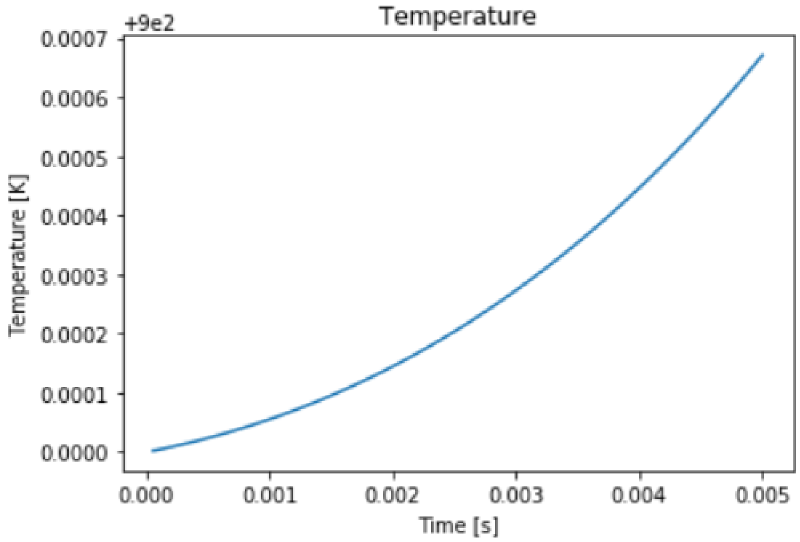
- Propane (C_3H_8)

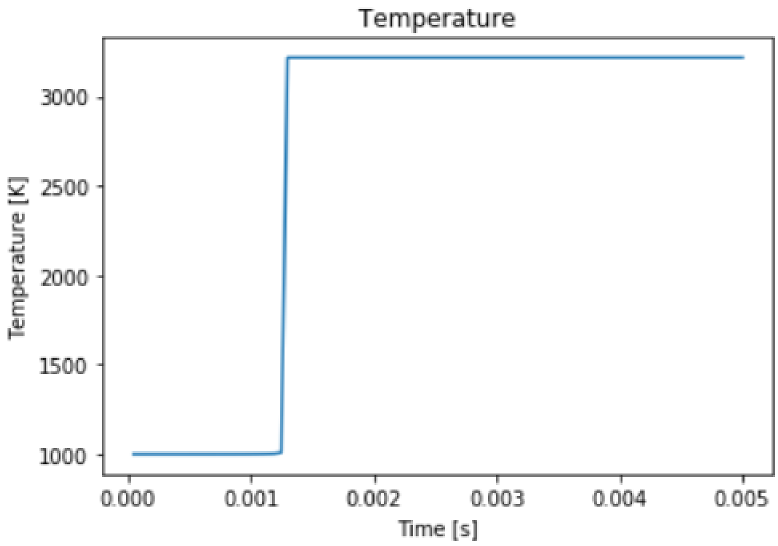






- Hydrogen (H_2)


Temperature
+9e2
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0.0000
Temperature [K]
0.000
0.001
0.002
0.003
0.004
0.005
Time [s]


Temperature
3000
2500
2000
1500
1000
Temperature [K]
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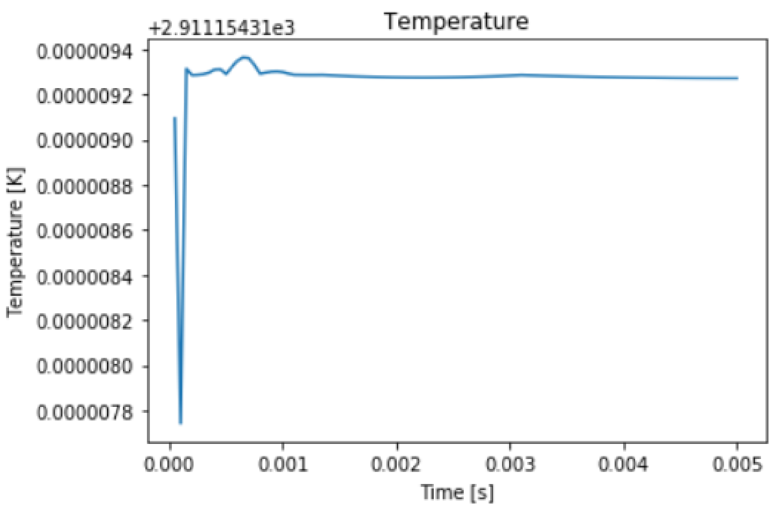
0.001
0.002
0.003
0.004
0.005
Time [s]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0.0000092
0.0000090
0.0000088
0.0000086
0.0000084
0.0000082
0.0000080
0.0000078
Temperature [K]
0.000
0.001
0.002
0.003
0.004
0.005
Time [s]

- Heat combustion

L.p	Initial conditions	Fuel	LHV [MJ/kg]	HHV [MJ/kg]
1.	T=298 [K], p=101325	CH4	50,026	55,512
2.		C3H8	46,352	50,344
3.		H2	119,959	141,788
4.	T=400 [K], p=1,5 [bar]	CH4	49,965	54,868
5.		C3H8	46,352	50,344
6.		H2	119,959	141,788
7.	T=600 [K], p=3 [bar]	CH4	49,886	52,521
8.		C3H8	46,304	49,872
9.		H2	120,469	139,98