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Computational Methods in Combustion

The influence of initial conditions on heat combustion and temperature of various fuels

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1 Introduction

The aim of this project is to run simulations of various fuels which undergoes complete combustion in oxygen at various initial conditions and to measure the outgoing heat of combustion and temperature during complete combustion.

2 Definitions

The heat of combustion is the energy liberated when a substance undergoes complete combustion in reaction with oxygen at constant pressure. The heat of combustion is typically presented in the form of heating value. Upon knowing the heating value of specific fuel we are able to predict how may energy from this fuel we can use in our engines. We devide the heating value to higher and lower heating values.

The lower heating value (LHV) (also known as net calorific value) of a fuel is defined as the amount of heat released by combusting a specified quantity (initially at 25°C) and returning the temperature of the combustion products to 150°C, which assumes the latent heat of vaporization of water in the reaction products is not recovered.

The higher heating value (HHV) (also known gross calorific value or gross energy) of a fuel is defined as the amount of heat released by a specified quantity (initially at 25°C) once it is combusted and the products have returned to a temperature of 25°C, which takes into account the latent heat of vaporization of water in the combustion products.

Mathematical corelation

$$HHV = LHV + H_v\left(\frac{n_{H20,out}}{n_{fuel,in}}\right)$$

H_v is the heat of vaporization of water,$n_{H20,out}$ is the moles of water vaporized and $n_{fuel,in}$ is the number of moles of fuel combusted

3 Model and initial conditions

Temperatures - the moel measures the temperatures of combustion of four different fuels. The modek is using a reactor with constant pressure and writing results every 0,00005 second in span of 0 to 0,005 second. the results are shown on plots.

Fuels

1. Methane (CH_4)
2. Propane (C_3H_8)
3. Hydrogen (H_2)
4. Ethane (H_2C_6)

Initial conditions

1. $T_1 = 298[K]$ $p_1 = 101325[Pa]$
2. $T_2 = 400[K]$ $p_1 = 2,5[atm]$
3. $T_3 = 500[K]$ $p_1 = 5[atm]$

Combustion reaction

- Methane (CH_4)

$$CH_4 + 2O_2 -> CO_2 + 2H_2O$$

- Propane (C_3H_8)

$$C_3H_8 + 5O_2 -> 3CO_2 + 4H_2O$$

- Hydrogen (H_2)

$$2H_2 + O_2 -> 2H_2O$$

- Ethane (H_2C_6)

$$2C_2H_6 + 7O_2 -> 4CO_2 + 6H_2O$$

4 Results

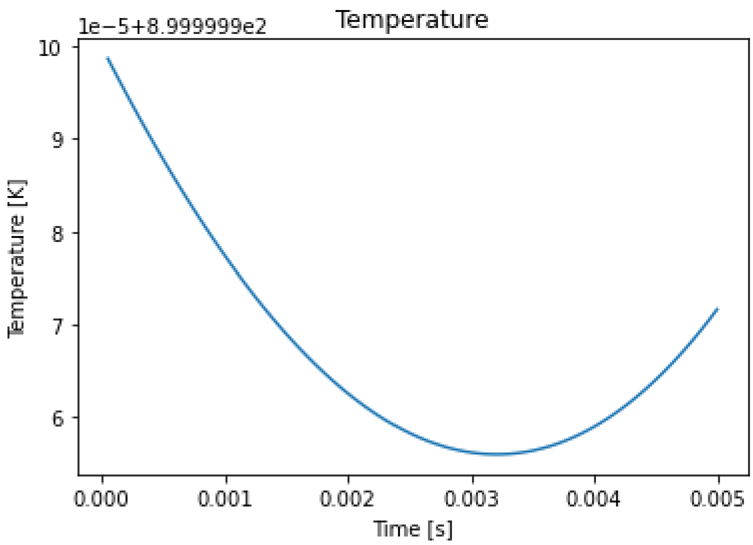

Figure 1: Methane $(CH_4), T_1, p_1$

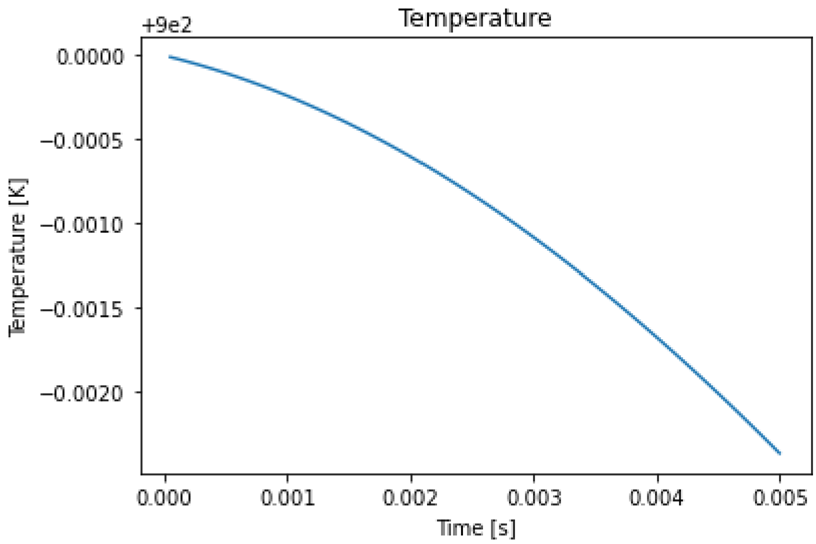

Figure 2: Propane $(C_3H_8), T_1, p_1$

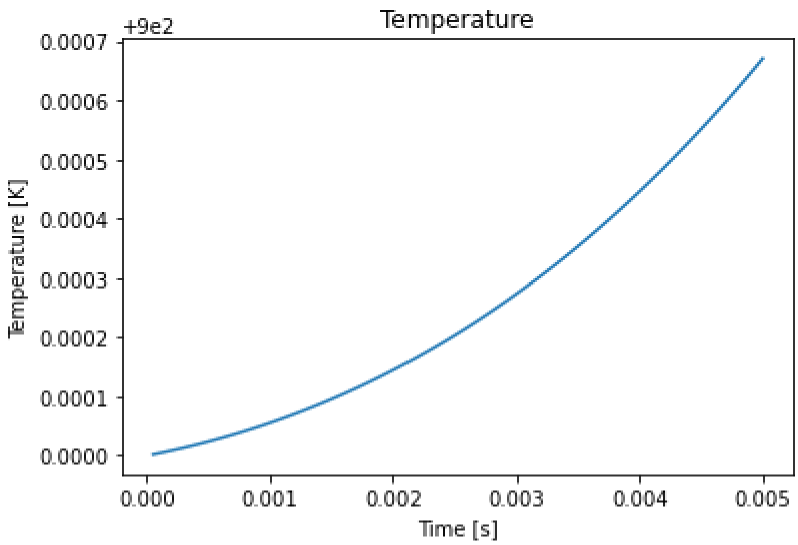

Figure 3: Hydrogen $(H_2), T_1, p_1$

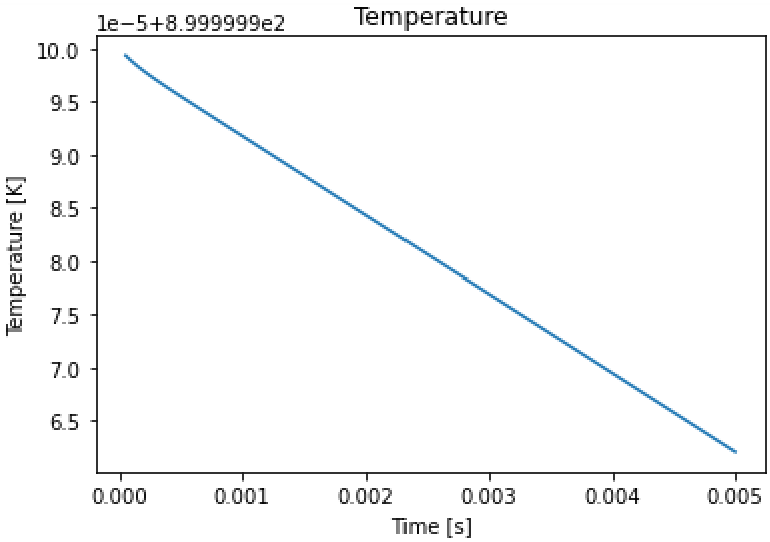

Figure 4: Ethane $(H_2C_6), T_1, p_1$

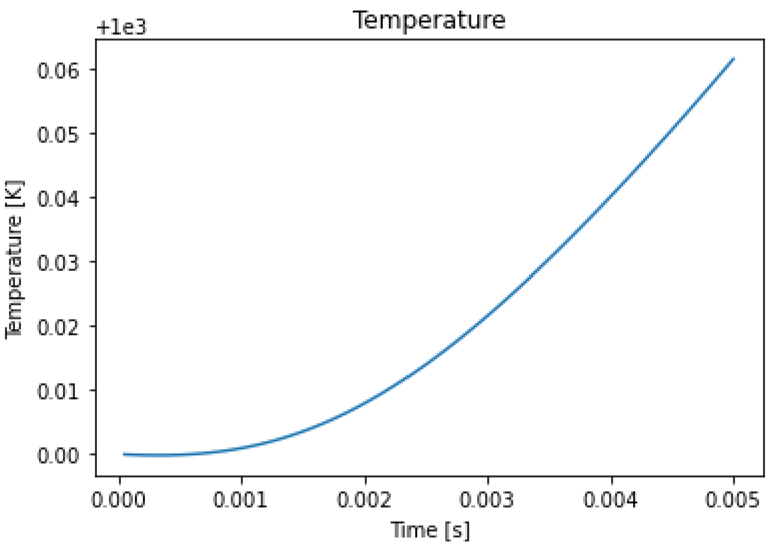

Figure 5: Methane $(CH_4), T_2, p_2$

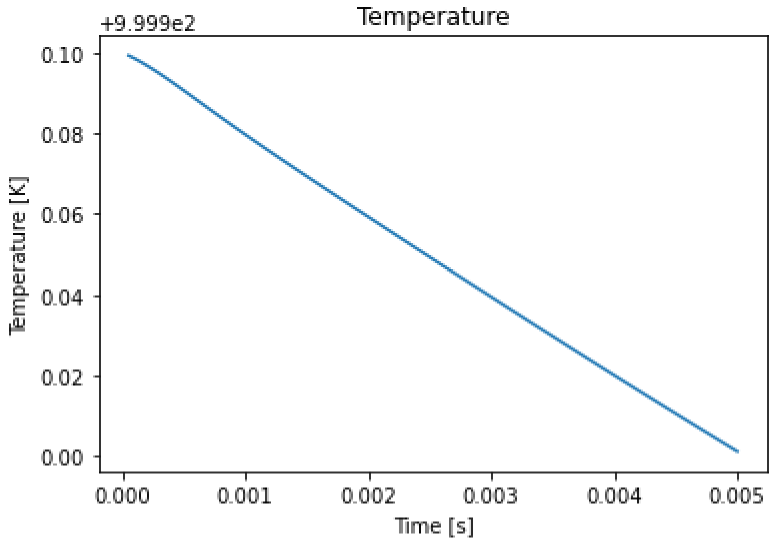

Figure 6: Propane $(C_3H_8), T_2, p_2$

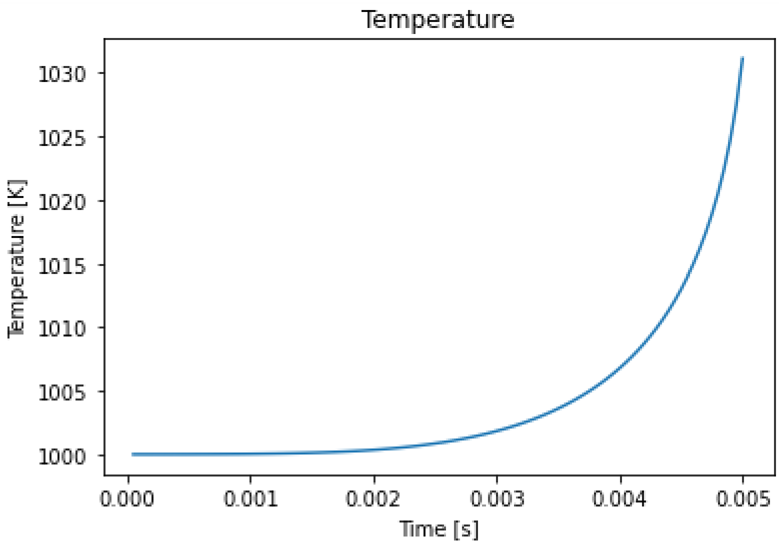

Figure 7: Hydrogen $(H_2), T_2, p_2$

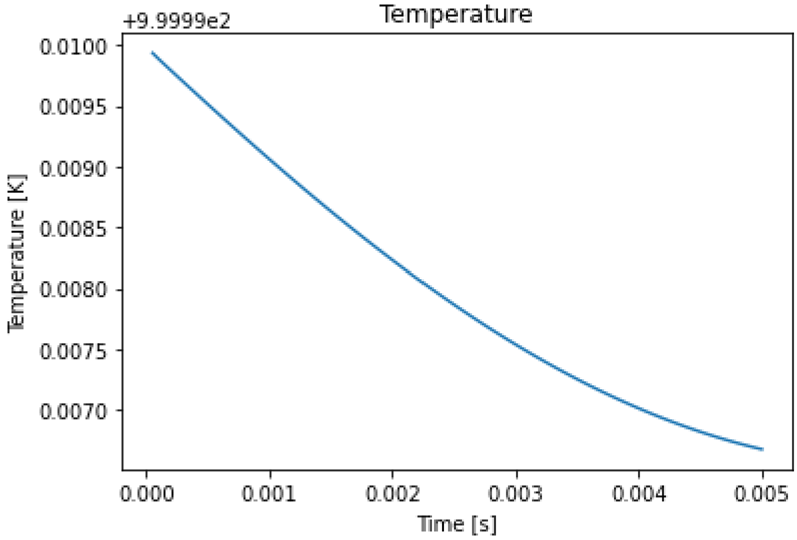

Figure 8: Ethane $(H_2C_6), T_2, p_2$

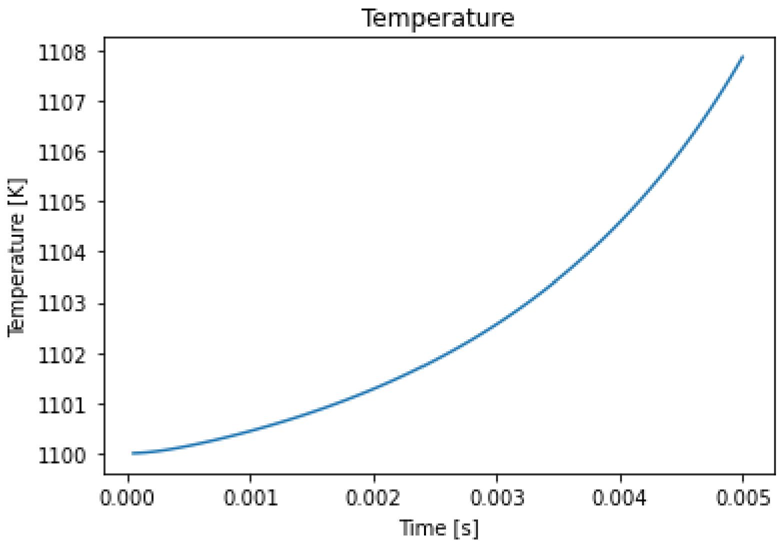

Figure 9: Methane $(CH_4), T_3, p_3$

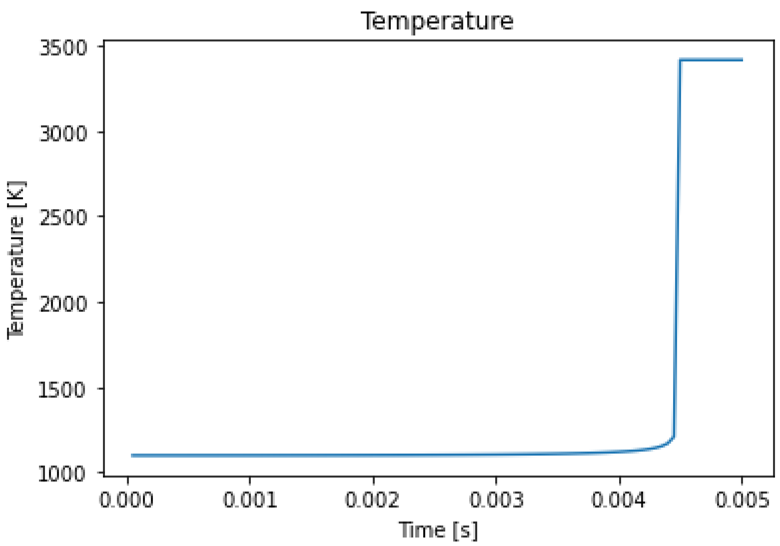

Figure 10: Propane $(C_3H_8), T_3, p_3$

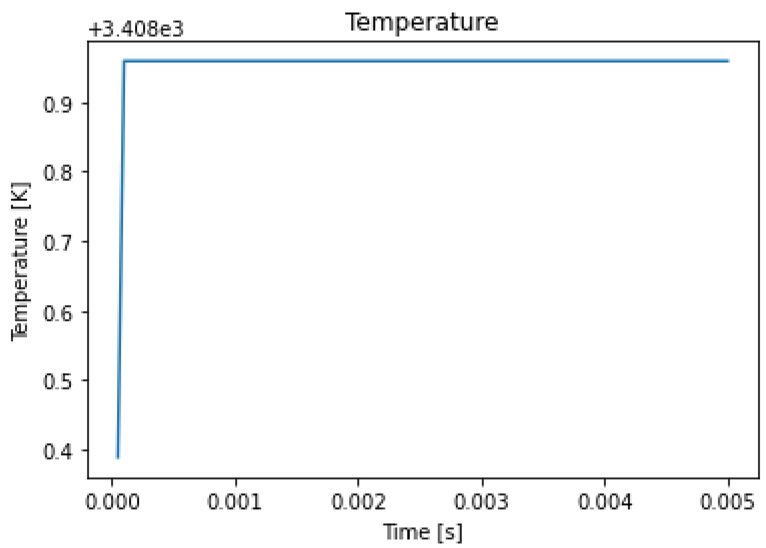

Figure 11: Hydrogen $(H_2), T_3, p_3$

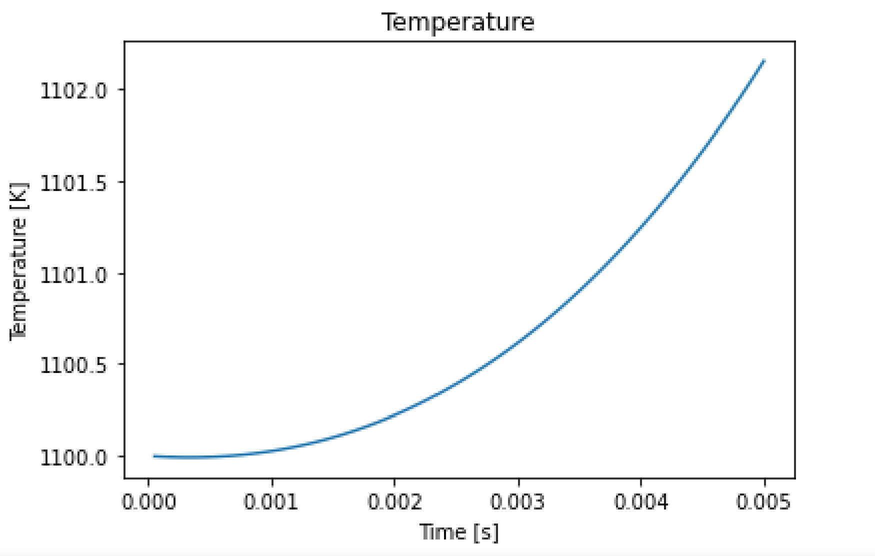

Figure 12: Ethane $(H_2C_6), T_3, p_3$

Fuel	T[K]	p[atm]	LHV [MJ/kg]	HHV [MJ/kg]
CH4	298	1	50,025	55,511
	400	2,5	49,964	54,867
	500	5	49,915	54,021
C3H8	298	1	46,352	50,343
	400	2,5	46,304	49,871
	500	5	46,277	49,265
H2	298	1	119,952	141,78
	400	2,5	120,462	139,971
	500	5	120,952	137,29
C2H6	298	1	47,511	51,501
	400	2,5	47,451	51,375
	500	5	47,413	50,699

Figure 13: HHV and LHV results