# COMPUTER MERHODS IN COMBUSTION

# REPORT

Influence of inlet air speed on combustion temperature and thrust in Cantera with comparison of the usage of two different fuels

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Warsaw 2021

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### 1 Introduction

This project was created to evaluate the influence of inlet air speed on combustion temperature and generated thrust using Cantera environment. Moreover in this project, an extra comparison of the usage of different fuels in the combustion simulation. Fuels chosed for calculations was gas ethane and gas methane.

Calculations were performed with following constant starting parameters:

- Stoichiometric methane air mixture or Stoichiometric ethane air mixture
- Volume of combustion chamber  $0.5 m^3$
- Air parameters for 4000 m altitude

Calculations of thrust in this project was made by usage of build-in Cantera method. Furthermore to initialize combustion process, hydrogen radicals was injected into the combustion chamber. This solution is recommended for investigated process by Cantera developers.

#### 2 Methods

#### 2.1 Mathematical model

For calculation purpose some simplifications has been made in models of inlet, combustion chamber and nozzle.



Figure 1: Simple model of adiabatic inlet, combustion chamber and adiabatic nozzle

Reactions simulated by Cantera environment are based on following equations with assumption that air consists of 21% of oxygen and 79% of Nitrogen:

$$CH_4 + 2\,O_2 + 7.52\,N_2 \xrightarrow{\ H\ } 2\,H_2O + CO_2 + 7.52\,N_2 \ \text{for methane}$$
 
$$2\,C_2H_6 + 7\,O_2 + 26.32\,N_2 \xrightarrow{\ H\ } 6\,H_2O + 4\,CO_2 + 26.32\,N_2 \ \text{for ethane}$$

Considering chemical equations posted above, the theoretical oxygen demand for combustion of methane and ethane in air was calculated.

$$\mu_{CH_4} = \frac{n_{O_2} + n_{N_2}}{n_{CH_4}} = \frac{2 + 7.52}{1} = 9.52 \left[ \frac{mol}{mol} \right]$$
 (1)

$$\mu_{C_2H_6} = \frac{n_{O_2} + n_{N_2}}{n_{CH_4}} = \frac{7 + 26.32}{2} = 16.67 \left[ \frac{mol}{mol} \right]$$
 (2)

During the calculations equivalence ratio was set to 1, which corresponds to the stoichiometric reaction.

Calculations were performed within 4 phases:

- 1 Calculation of boundary air parameters according to specified altitude and Mach number.
- 2 Calculation of air, fuel and igniter in combustion chamber filled initially with air.
- 3 Calculation of steady-star temperature of methane and ethane combustion.
- 4 Calculation of jet engine thrust.

Following the first phase of calculation starting air parameters were estimated according to International Standard Atmosphere:

$$T = T_0 - 6, 5 \cdot H \ (H \ in \ km) \tag{3}$$

$$p = p_0 \cdot \left(1 - \frac{H}{44300}\right)^{5,256} \tag{4}$$

$$\rho = \rho_0 \cdot \left(1 - \frac{H}{44300}\right)^{4,256} \tag{5}$$

Then velocity of air was calculated according to Mach number and local speed of sound. Relevant formula posted below:

$$v = M \cdot a = M \cdot \sqrt{\kappa \cdot R \cdot T} \tag{6}$$

where:

$$\kappa = \frac{c_v}{c_n} \tag{7}$$

Next the air was set to higher enthalpy caused by supersonic flow, also total pressure of air was estimated:

$$h_1 = h_0 + \frac{v^2}{2} \tag{8}$$

$$p_1 = p_0 \cdot \left(\frac{T}{T_0}\right)^{\frac{n}{n-1}} \tag{9}$$

Mass of air flowing through the 'engine' was calculated following formula number (10), which is assumed to be the most convenient in this case:

$$m_a \left[ \frac{\text{kg}}{\text{m}} \right] = \mu \cdot \rho_a \cdot A \tag{10}$$

Where area (A) was set to  $m^2$ .

Next fuel mass flow was estimated by formula below:

$$m_f \left[ \frac{\text{kg}}{\text{m}} \right] = \frac{m_{\text{a}} \cdot \phi}{\mu} \tag{11}$$

With mass flows of fuel and air calculated, next step is calculation of total mas flow ratio:

$$m = m_a + m_f \tag{12}$$

Finally velocity of outlet air and thrust were calculated:

$$v_e \left[ \frac{\mathbf{m}}{\mathbf{s}} \right] = \sqrt{2 \cdot c_p \cdot T_0 \cdot \left( 1 - \frac{T}{T_0} \right)} \tag{13}$$

$$T[N] = m \cdot v_e \cdot (v_{\varepsilon} - v_0) - \frac{m}{\rho} \cdot (p_{\varepsilon} - p_1)$$
(14)

Additionally, for better comparison the propulsion efficiency was estimated by formula below:

$$\eta = \frac{2}{1 + \frac{v_n}{v_b}} \tag{15}$$

#### 2.2 Code description

The code is build from there major parts. First part contains calculation of air parameters according to Mach number International Standard Atmosphere. At the beginning temperature, density, pressure were set to static values calculated according to formulas presented in previous paragraph. Then air was set using changed enthalpy and total pressure.

Initially combustion chamber was filled with air with parameters evaluated for a certain Mach number.

Second part of the code is responsible for chemical reaction simulation, in this case combustion. Whole simulation was competed with aim to get steady state temperature. It is achieved by supplying the combustion reactor with air at stagnation temperature of fuel at 300K and a Hydrogen radical that initiates the ignition. In this solution Hydrogen radicals temperature was also set to 300 K.

Hydrogen mass flow ratio was delivered as function of time, which is based on normal distribution:

$$\lambda_t = a \cdot e^{\frac{-(t - t_0)^2}{2 \cdot f w^2}} \tag{16}$$

where a is amplitude and fw is standard deviation. Parameters were chosen to produce a quick injection at second second of the process.

Combustion was set to last for 4 seconds. This duration of simulation was estimated by previous trails and turned out to be enough time to get steady state.

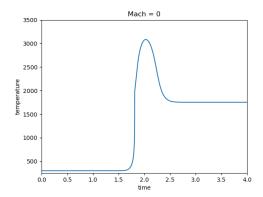
The last part consist of calculating thrust and plotting. Some results were printed into the text file and then some plots were edited in MS Excel.

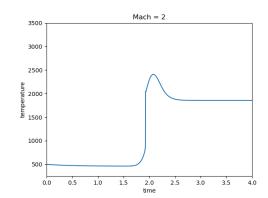
Cantera functions used in this project were:

- Reservoirs for air, fuel, igniter and exhaust.
- Reactor for combustion chamber.
- Valve for outlet from reactor.
- Mass flow controller for setting mass flow rate to the reactor.

Value of valve pressure drop was set to 1, which provides pressure on outlet with the same value as pressure of inlet.

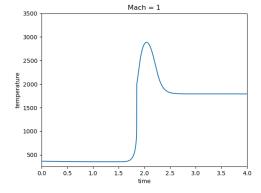
#### 3 Results





CH<sub>4</sub> and Mach 0

Figure 2: Temperature as function of time for Figure 4: Temperature as function of time for CH<sub>4</sub> and Mach 2



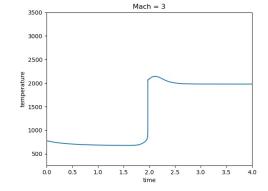
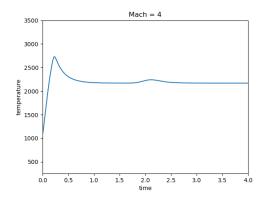


Figure 3: Temperature as function of time for Figure 5: Temperature as function of time for CH<sub>4</sub> and Mach 1

CH<sub>4</sub> and Mach 3



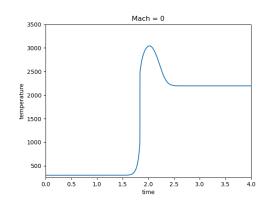
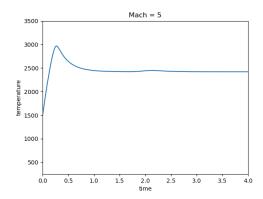
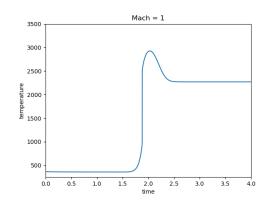


Figure 6: Temperature as function of time for Figure 9: Temperature as function of time for CH<sub>4</sub> and Mach 4

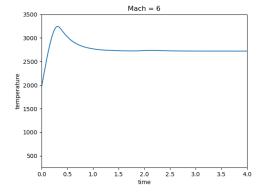
 $C_2H_6$  and Mach 0





 $CH_4$  and Mach 5

Figure 7: Temperature as function of time for Figure 10: Temperature as function of time for  $C_2H_6$  and Mach 1



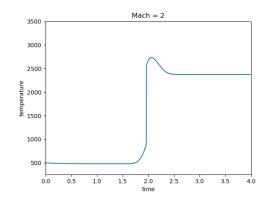
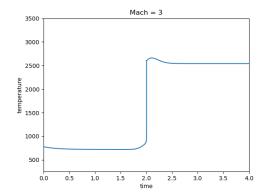
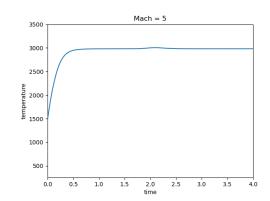


Figure 8: Temperature as function of time for Figure 11: Temperature as function of time for CH<sub>4</sub> and Mach 6

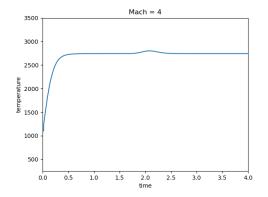
 $C_2H_6$  and Mach 2

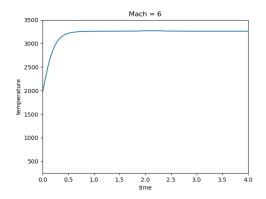




 $C_2H_6$  and Mach 3

Figure 12: Temperature as function of time for Figure 14: Temperature as function of time for  $C_2H_6$  and Mach 5





 $C_2H_6$  and Mach 4

Figure 13: Temperature as function of time for Figure 15: Temperature as function of time for  $C_2H_6$  and Mach 6

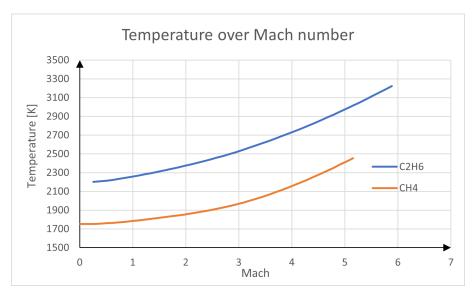


Figure 16: Steady state temperature as function of Mach number

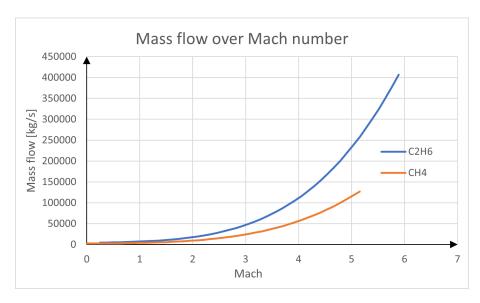


Figure 17: Mass flow as function of Mach number

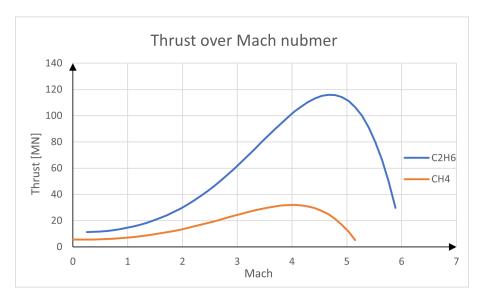


Figure 18: Thrust as function of Mach number

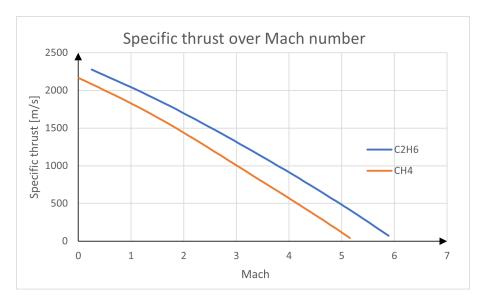


Figure 19: Specific thrust as function of Mach number

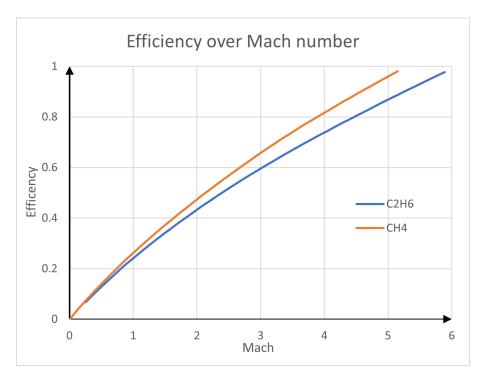


Figure 20: Efficiency as function of Mach number

# 4 Analysis with fuel comparison

Figures 2 - 15 shows temperature over the time of simulation for different Mach numbers.

First focusing in graphs for  $CH_4$ , Up to Mach 3 the temperature of air flowing through chamber was too low to initiate combustion, so hydrogen radicals acting as igniter was introduced. With igniter as initiator of combustion reaction peak temperature appeared around second second of simulation (quickly after igniter injection). Highest peak temperature is achieved at Mach 0. Nonetheless steady state temperature grow with Mach number

After Mach 3 the combustion reaction was initiated without igniter. Moreover it stared almost immediately after the simulation was launched. Steady state temperature was achieved around end of the first minute of the simulation. On the contrary to the igniter initiated combustion reactions, in self initiated reactions peak temperature rise with Mach number. However the steady state temperature also grow with Mach number.

Then analyzing closely second fuel  $(C_2H_6)$  charts until Mach 3 same trends can be spotted. Nevertheless after Mach 3 totally different type of reaction has been observed. Steady state temperature is equal to the first peak temperature and is growing with Mach number, the other thing that has been spotted is a little peak at second second where igniter is injected.

The anomaly might appear because the combustion reaction is still ongoing through the estimated four seconds. That aspect of simulation may indicate appearance of uncontrolled explosion, which is obviously excluding further application in jet engine. With that knowledge in further comparison of fuels, cases over Mach 3 were abandoned.

Figures 16 - 20 present comparison of certain parameters that can help with evaluation of fuels.

At figure 16 we can spot huge difference between steady state temperature, temperature for  $CH_4$  is nearly about 500 K lower than temperature for  $C_2H_6$ .

Then analyzing the mass flow ratio over Mach number, there is visible that the  $C_2H_6$  curve has higher growth ration than  $CH_4$  curve. Nearly doubling Mass flow around 3 Mach.

Further going to calculated thrust, It is clear that combustion of  $C_2H_6$  generates more thrust with much higher growth ration for Mach numbers around 2 and 3. Moreover Specific thrust for  $C_2H_6$  is also bigger than specific thrust for  $CH_4$ .

However efficiency chart shows us that application of  $CH_4$  as a fuel is more efficient than  $C_2H_6$ . It is mostly due to the higher mass flow required to complete complete combustion reaction with stoichiometric ratio.

## 5 Summary

To conclude  $CH_4$  is more efficient fuel than  $C_2H_6$ , despite ethane produces more specific thrust. Nevertheless application of ethane as jet fuel may be useful for more thrust requiring purposes. Both fuels operates on high temperature levels so there would be no need of advanced engine modifications to adapt methane engine to ethane powered engine. However the results achieved after Mach 3 are worrying and should be further investigated.

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6	Temperature as function of time for $CH_4$ and Mach $4 \ldots 6$
7	Temperature as function of time for $CH_4$ and Mach 5
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19	Specific thrust as function of Mach number
20	Efficiency as function of Mach number

# 6 References

- $\bullet \ \ https://web.mit.edu/16.unified/www/FALL/thermodynamics/notes/node111.html$
- http://bcpw.bg.pw.edu.pl/Content/4566/03sws wielkosci.pdf
- http://www.cantera.org/docs/sphinx/html/cython/examples/reactors combustor.html
- $\bullet \ \, https://github.com/KasiaPo/MKWS$
- http://fisicaatmo.at.fcen.uba.ar/practicas/ISAweb.pdf