Metody Komputerowe w Spalaniu

Detonation speed of mixture for different initial temperature and pressure

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1. Introduction

The purpose of the project was to compare detonation speed of three different mixture:

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

Depends of three different initial conditions:

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

Calculations were performed using SDToolbox under Cantera. The results of the calculations are plots which showing influence of initial conditions on CJ detonation speed.

2. Mathematic model

The stoichometric reaction of complete combustion

- 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)

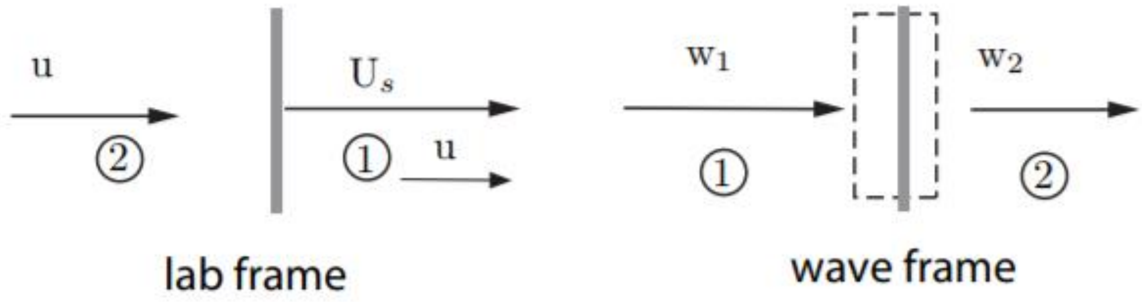
$$2H_2 + O_2 \rightarrow 2\ H_2O$$

Chapman-Jouguet (CJ) detonation. This is the limiting case of the minimum wave speed for the supersonic solutions to the jump conditions with exothermic reactions. The Chapman-Jouguet solution is often used to approximate the properties of an ideal steady detonation wave.

The resulting relationships are the conservation of:

- mass - $\rho_1 w_1 \;=\; \rho_2 w_2$
- momentum - $P_1 + \rho_1 {w_1}^2 = P_2 + \rho_2 {w_2}^2$
- energy - $h_1 + \frac{{w_1}^2}{2} = h_2 + \frac{{w_2}^2}{2}$

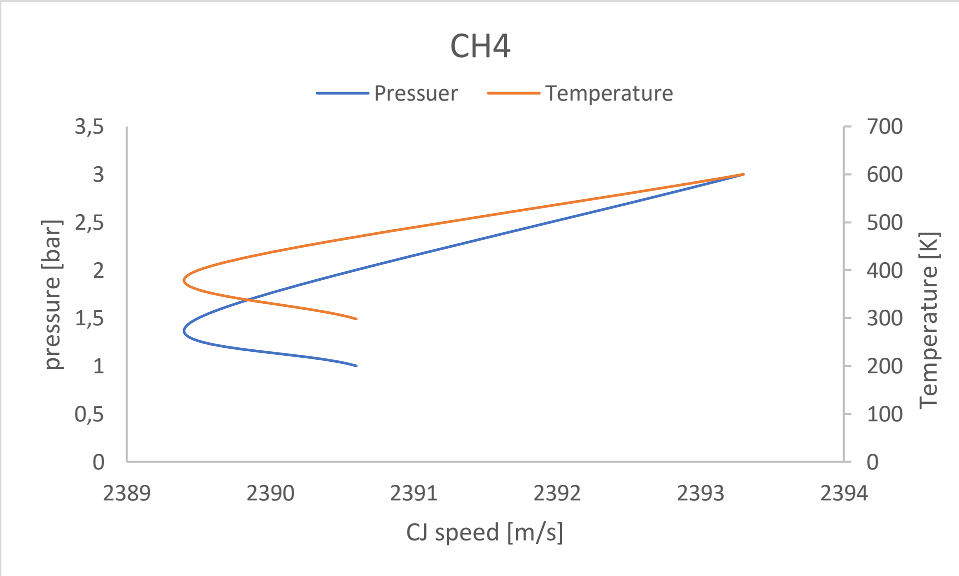
These equations apply equally to moving and stationary waves as well as to oblique waves as long as the appropriate transformations are made to the wave-fixed coordinate system

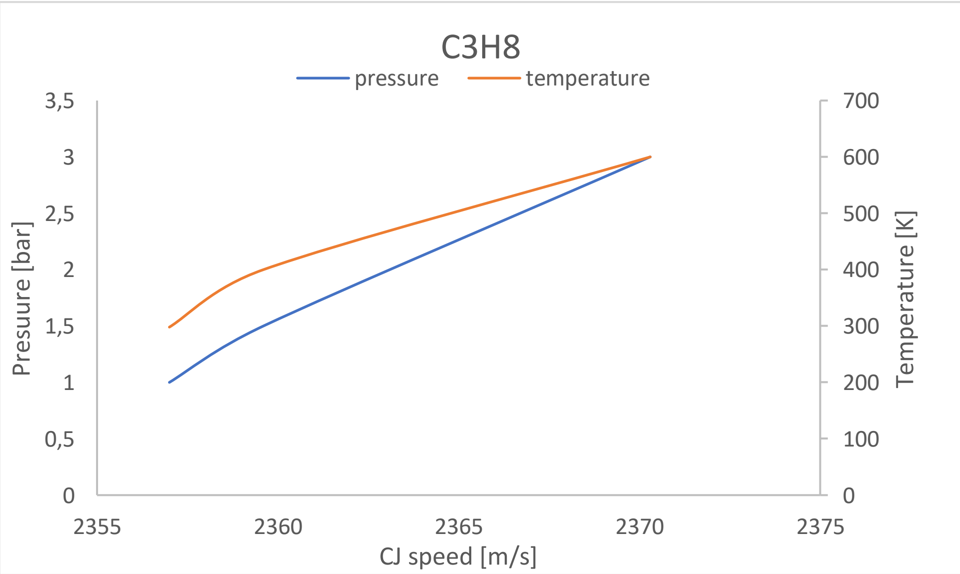


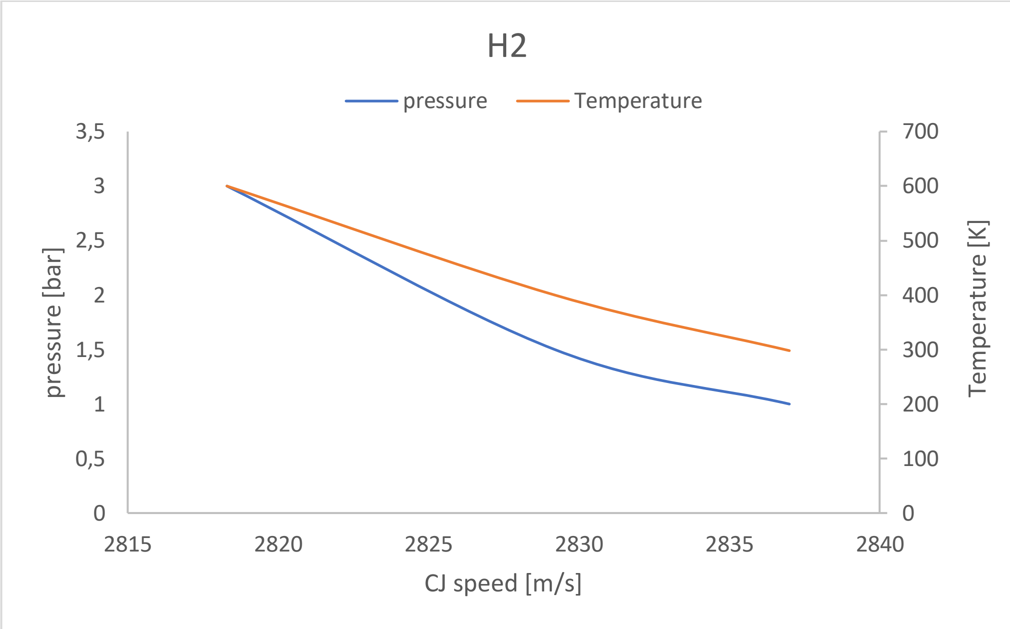
$$w_1 = U_s - u_1$$
$$w_2 = U_s - u_2$$

3. Results

L.p	Initial conditions	Fuel	CJ speed [m/s]
1.	T=298 [K], p=101325	CH4	2390,6
2.		C3H8	2357,5
3.		H2	2837,0
4.	T=400 [K], p=1,5 [bar]	CH4	2389,5
5.		C3H8	2359,6
6.		H2	2829,2
7.	T=600 [K], p=3 [bar]	CH4	2393,3
8.		C3H8	2370,3
9.		H2	2818,3







4. Conclusion

- The initial parameters pressure and temperature have influence on detonation speed
- The value of detonation speed is various for different mixtures
- The higher value of CJ speed definitely has a mixture of hydrogen and oxygen, but also only this mixture has decreasing tendency of CJ speed
- The speed of detonation for mixture of CH4 and C3H8 is increasing with higher value of pressure and temperature, which is different tendency with compere to H2
- From initial conditions 1 to initial condition 2, the CJ speed of CH4 has a small drop
- Different Initial conditions used in this project cause small changes of CJ speed. The higher changes are in hydrogen and oxygen mixture and they are around 18 [m/s]. In rest mixtures changes are smaller, for C3H8 – 15 [m/s] and for CH4 about 5 [m/s]

5. References

- mgr inz. Agnieszka Jach - Presentation “Wprowadzenie do Shock & Detonation Toolbox”
- S. Browne, J. Ziegler, and J. E. Shepherd “Numerical Solution Methods for Shock and Detonation Jump Conditions”
- https://en.wikipedia.org/wiki/Chapman%E2%80%93Jouguet_condition