Chapman - Jouguet conditions in methane-oxygen mixtures

Computational methods in combsution

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1 Introduction

This report presents a study of the Chapman-Jouguet conditions in various metahne-oxygen mixtures. The calculations were performed in SDToolbox based on Cantera, using $gri30\_highT.cti$ mechanism of kinetics and two functions: "CJSpeed" - which calculate velocity of propagation detonation wave and "Postshock" - to compute total parameters behind wave.

2 Mathematical model

The solver is based on 1-dimensional model of detonation, proposed by Chapman and Jouguet. This model treats detonation wave as discontinuity in fuel-oxidier mixture flow. Combustion is simplified to adding heat on wave.

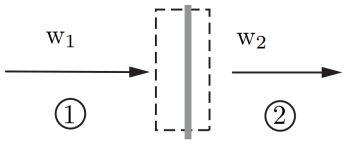

Figure 1: Idea of wave-fixed coordinates system. Index 1 denotes parameters before shockwave, while 2 denotes parameters behind the shockwave.

The principle of conservation of mass, momenteum and energy is fulfilled:

$$\rho_1 w_1 = \rho_2 w_2 \tag{1}$$

$$p_1 + \rho_1 w_1 u_1 = p_2 + \rho_2 w_2 u_2 \tag{2}$$

$$\frac{1}{2}w_1^2 + \frac{\kappa}{\kappa - 1}\frac{p_1}{\rho_1} = \frac{1}{2}w_2^2 + \frac{\kappa}{\kappa - 1}\frac{p_2}{\rho_2} + H \tag{3}$$

where:
p - pressure
ρ - density
w - velocity of shockwave propagation
u - velocity of gas
H - heat coming from chemical reaction

The total parameters behind the detonation wave are computed from equations:

$$p_2 = p_1 + \rho_1 \omega_1^2 (1 - \frac{\rho_1}{\rho_2}) \tag{4}$$

$$h_2 = h_1 + \frac{1}{2}\omega_1^2 (1 - (\frac{\rho_1}{\rho_2})^2) \tag{5}$$

The equation represnting Rayleigh line:

$$p_2 = p_1 - \rho_1^2 \omega_1^2 (v_2 - v_1) \tag{6}$$

The eqaution of Hugoniot curve:

$$h_2 = h_1 + \frac{(p_2 - p_1)(v_2 + v_1)}{2} \tag{7}$$

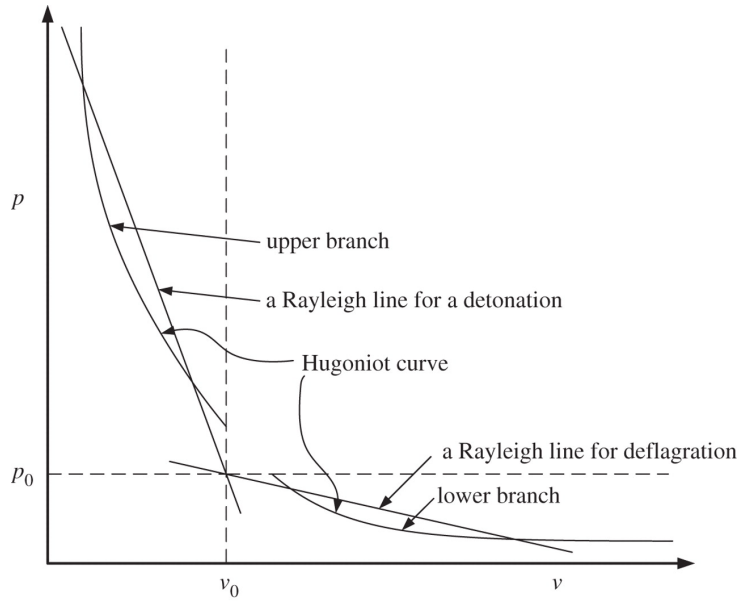

Figure 2: Traditional pressure–volume (p – v) diagram showing the Hugoniot curve with possible states of deflagrations and detonations.

The angle of Rayleigh line shows if detonation occrus and it represents speed of shock-wave.

3 Results

The calculations were carried out for 3 cases of initial thermodynamics condition:

I - $\phi = 1\ const$, $T = 300K\ const$, $p \in < 1, 10 > atm$

II - $\phi = 1\ const$, $P = 1atm\ const$, $T \in < 273, 2000 > K$

III - $p = 1\ atm\ const$, $T = 273K\ const$, $\phi \in < 0.1, 10.0 >$

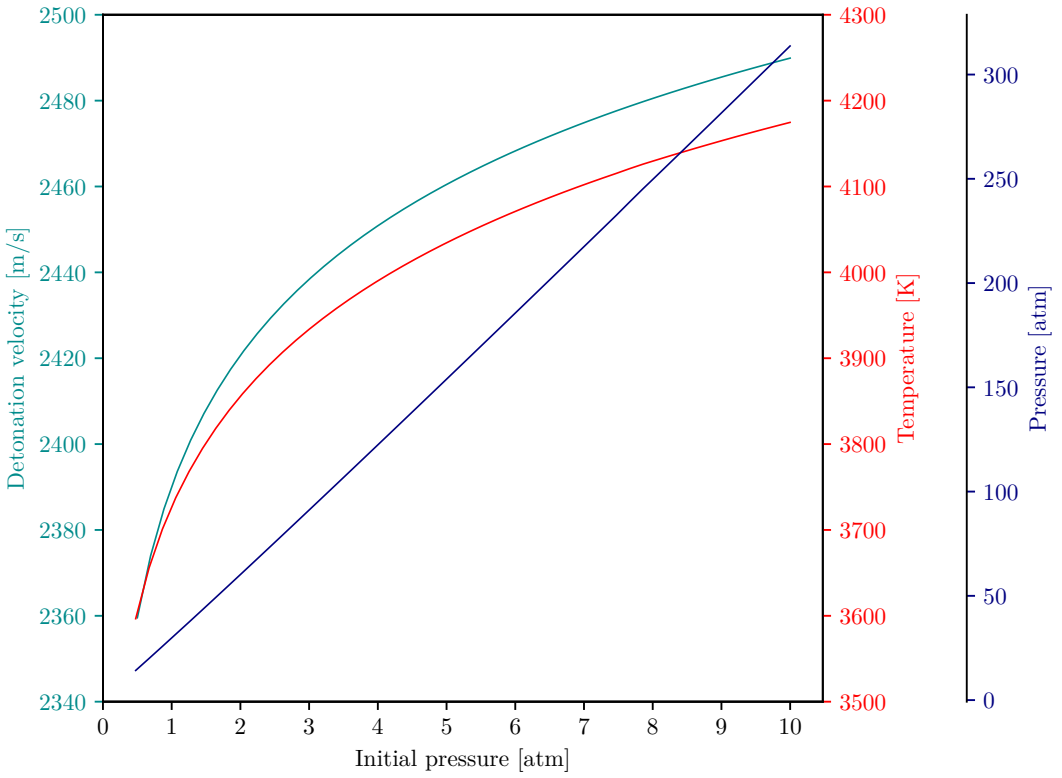

Figure 3: C-J detonation parameters for $CH_4 + O_2$ mixture in function of initial pressure

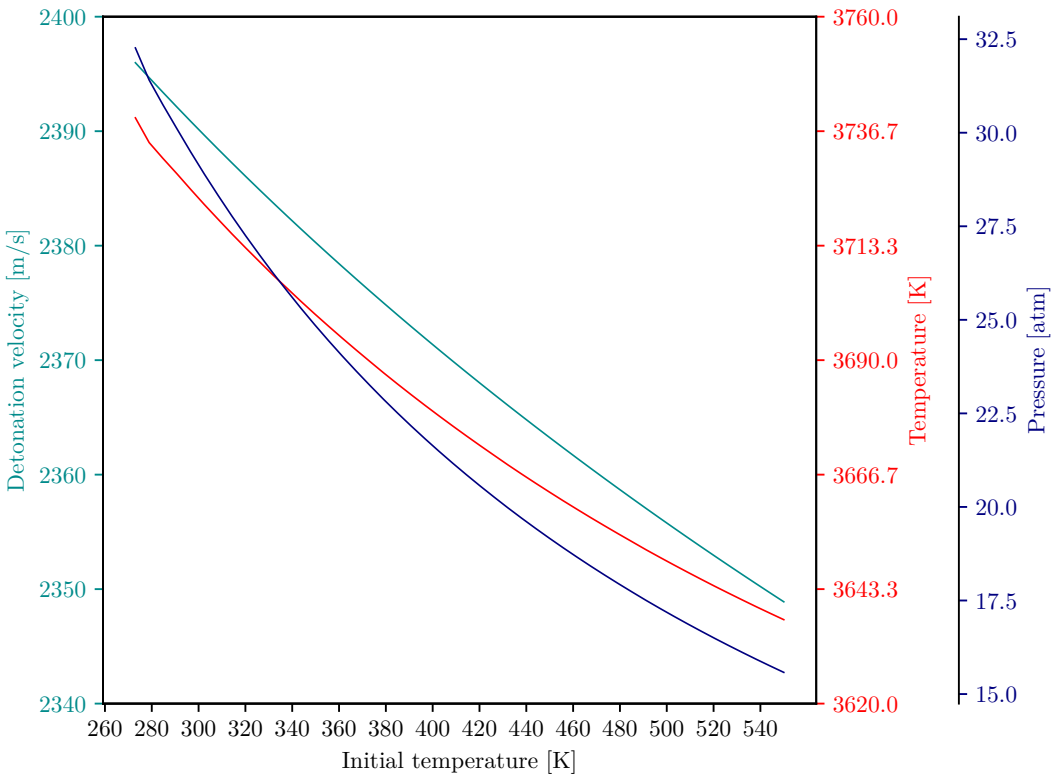

Figure 4: C-J detonation parameters for $CH_4 + O_2$ mixture in function of initial temperature

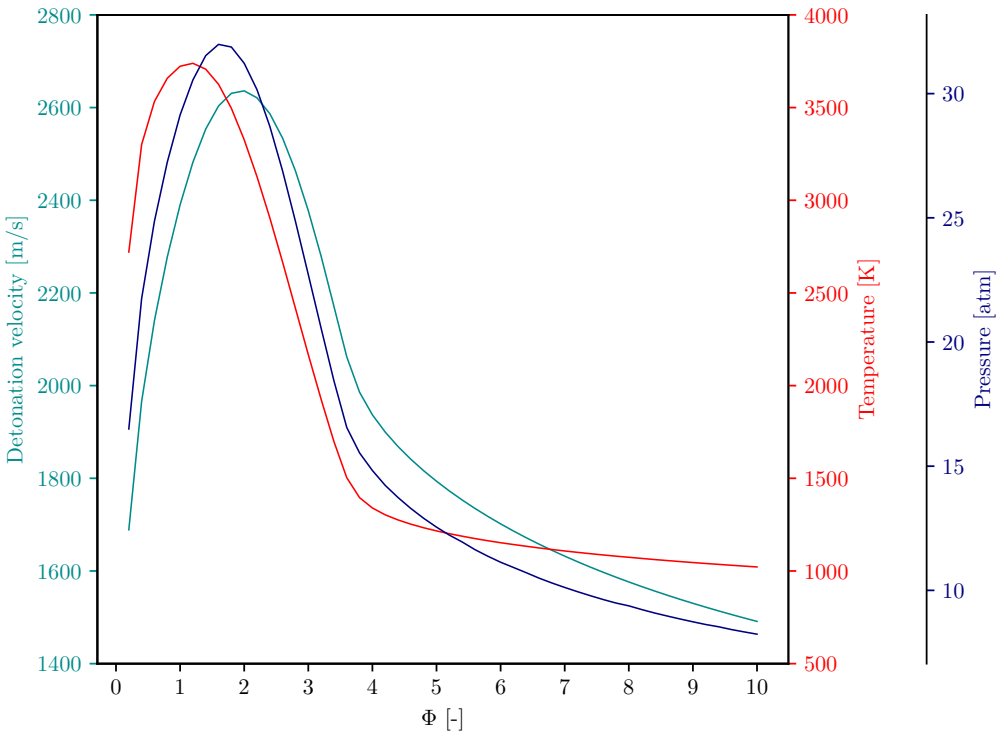

Figure 5: C-J detonation parameters for $CH_4 + O_2$ mixture in fucntion of ϕ

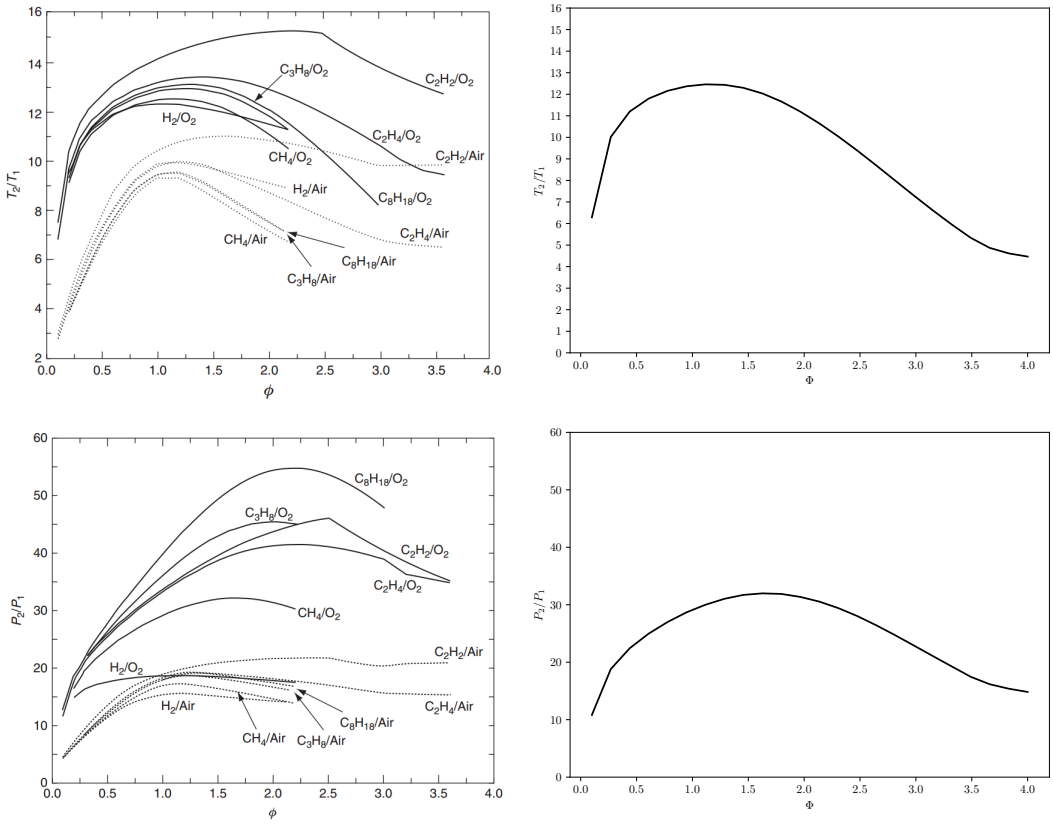

Figure 6: Comparison of CJ state parameters to initial parameters ratio between data form this study (right side) and *Combsution*[3](left side)

4 Summary

The parameters of Chapman-Jouguet detonation are strongly linked with initial parameters. Moreover total pressure and total temperature behind the wave depends from velocity of propagation with similiar tendency.

The maximum C-J detonation speed is reached for value around $\phi = 2$. All other parameters also reached their peak around this value. With rising of initial pressure the parameters beihnd the wave also increase. When initial temperature is variable the tendency is oppostie.

References

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[2] The physics, chemistry and dynamics of explosions, *Elaine S. Oran, Forman A. Williams*, Phil. Trans. R. Soc. A (2012) 370, 534–543

[3] Combusiton, *Irvin Glassman, Richard A. Yetter*, ISBN: 978-0-12-088573-2