Chapman - Jouguet conditions in methane-hydrogen-air mixtures

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1 Introduction

This report presents a study of the CJ conditions in various propane - hydrogen - oxygen mixtures. The calculations were performed in SDToolbox, using "wang_highT" mechanism of kinetics and two functions: "CJSpeed" and "Postshock_eq".

2 Mathematical model

The solver is based on the simpliest, 1-dimensional model of detonation, proposed by Chapman and Jouguet around 1900. It treats the detonation wave as a discontinuity in flow, allowing the use of three basic conservation laws: mass, momentum and energy.

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

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

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

Where:
p - pressure
ρ - density
w - velocity of shockwave propagation
u - velocity of gas
H - heat coming from chemical reaction
Index 1 denotes parameters before shockwave, while 2 denotes parameters behind the shockwave.

Knowing H of a given mixture(from Cantera), one can calculate all the other thermodynamic parameters.

3 Results

The initial thermodynamic conditions of a mixture are:
p = 1 bar
T = 300K

Five propane concentrations were taken into consideration - 0%, 3%, 6%, 9% and 12%. The concentration of hydrogen varies constantly from 5 to 80%. It was hard to determine the ignition limits for this mixture, so the results are presented for whole spectrum of concentrations.
The following plots show three basic parameters of a detonative combustion - CJ speed, pressure and temperature behind the wave.

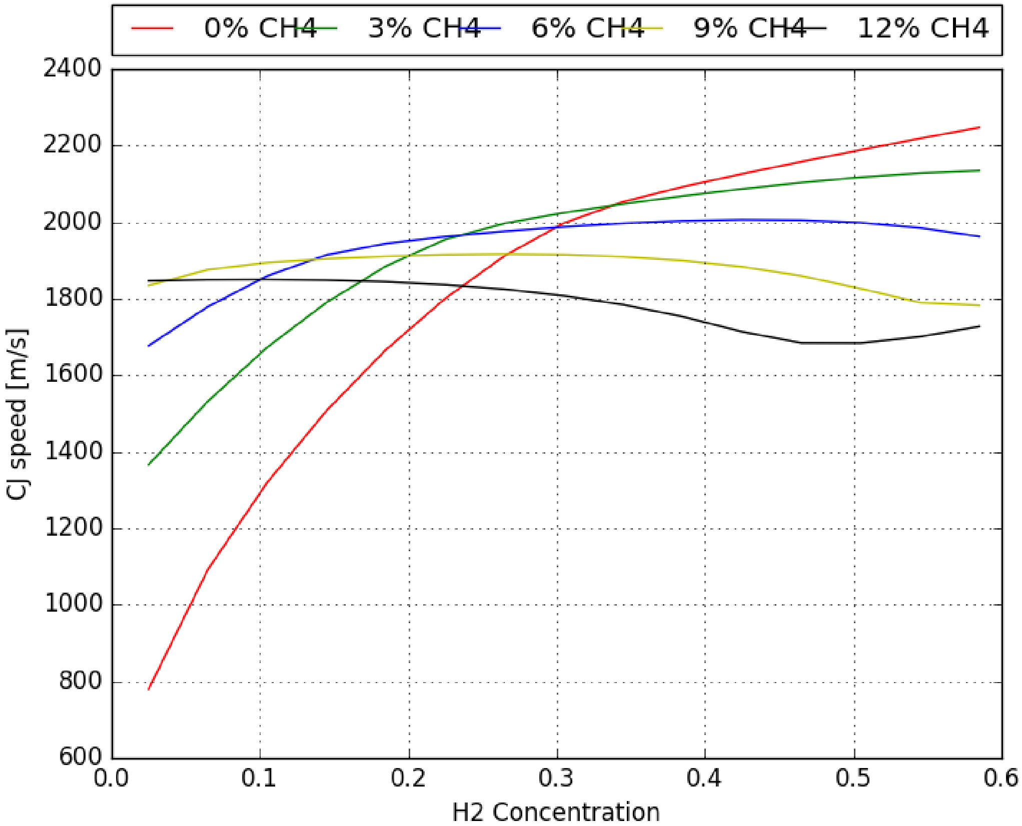

Figure 1: . Chapman Jouguet velocity vs H2 and CH4 concentration

What can be read from Fig 1 is that there is no maximum CJ speed for a pure hydrogen - air mixture. As the amount of methane increases, the point of maximum moves to the lower hydrogen concentrations. The chart shows correlation between methane, hydrogen concentration and pressure. For higher methane concentration there is rise in pressure, up to 17.2 bar.

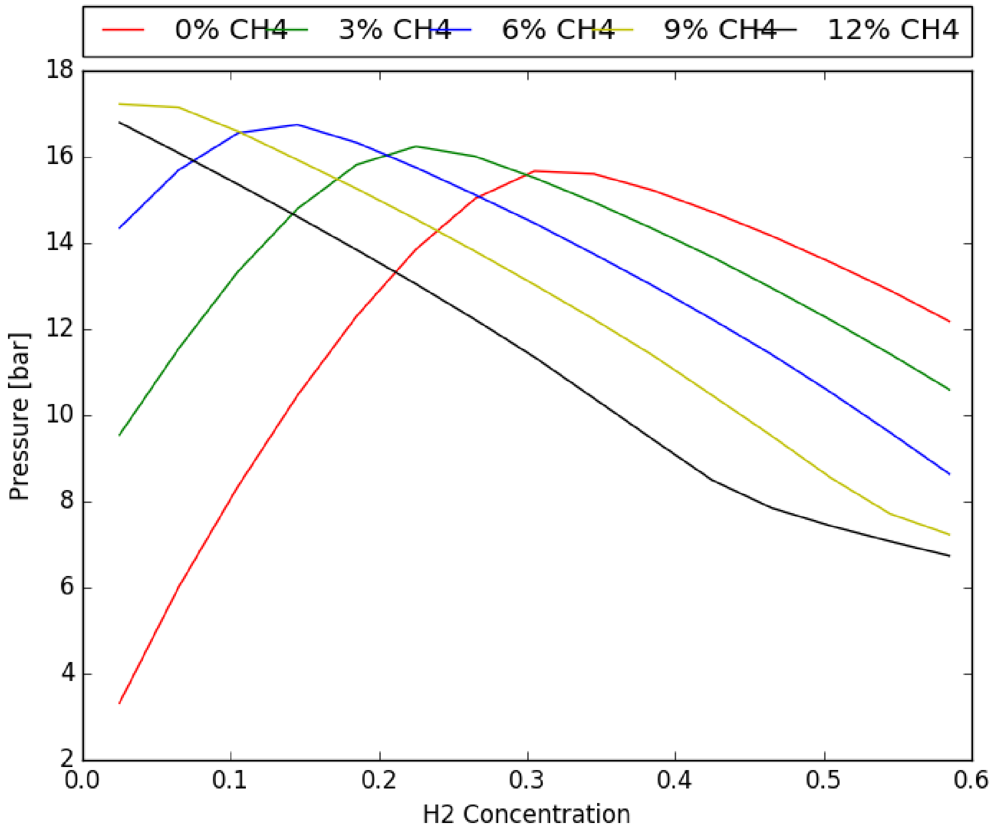

Figure 2: . Chapman Jouguet pressure vs H2 and CH4 concentration

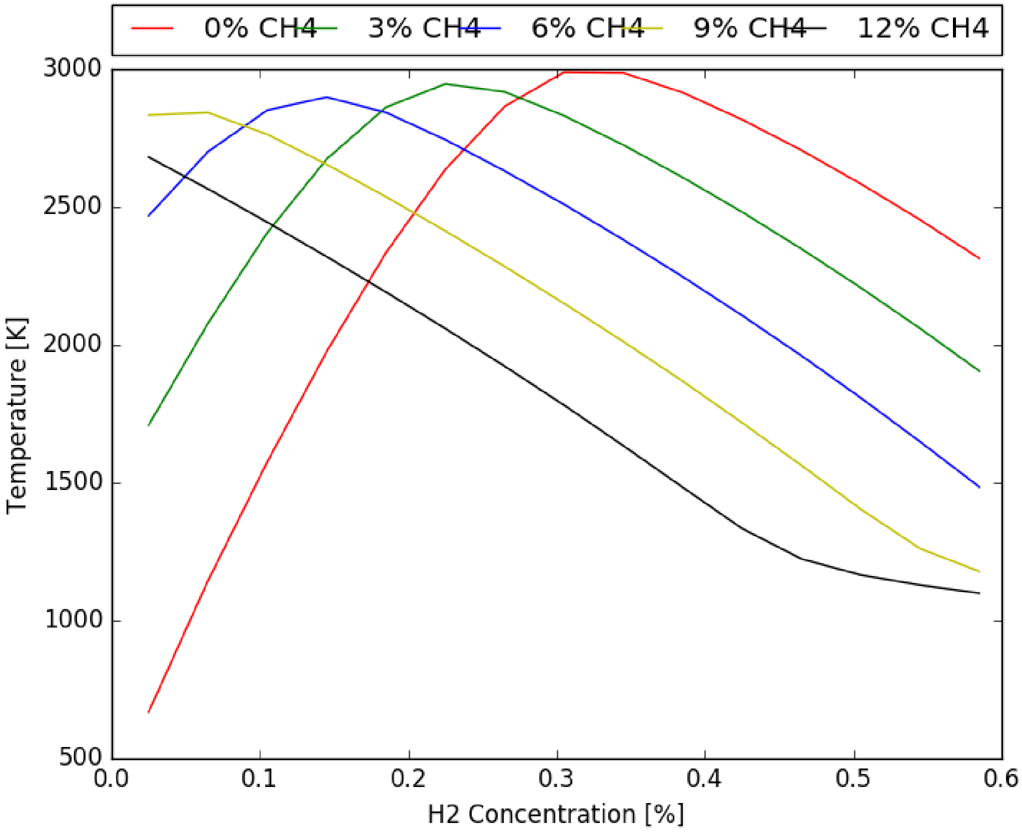

Figure 3: . Chapman Jouguet temperature vs H2 and CH4 concentration

The chart shows correlation between methane, hydrogen concentration and temperature. For higher methane concentration there is drop in temperature, from 3000K to 2700K.

4 Summary

- The CJ speed for pure hydrogen-air mixtures increases with hydrogen concentration
- With methane added, the maximum starts to appear
- For highest and lowest methane concentration pressure differs 10%, whilst temperature only 3%. - Maximum pressure increases for higher methane concentration and lower hydrogen concentration, whilst maximum temperature increases for lower methane concentration and higher hydrogen concentration.