Chapman - Jouguet conditions in propane-hydrogen-air mixtures

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Contents

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%, 5%, 10%, 15% and 20%. 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.

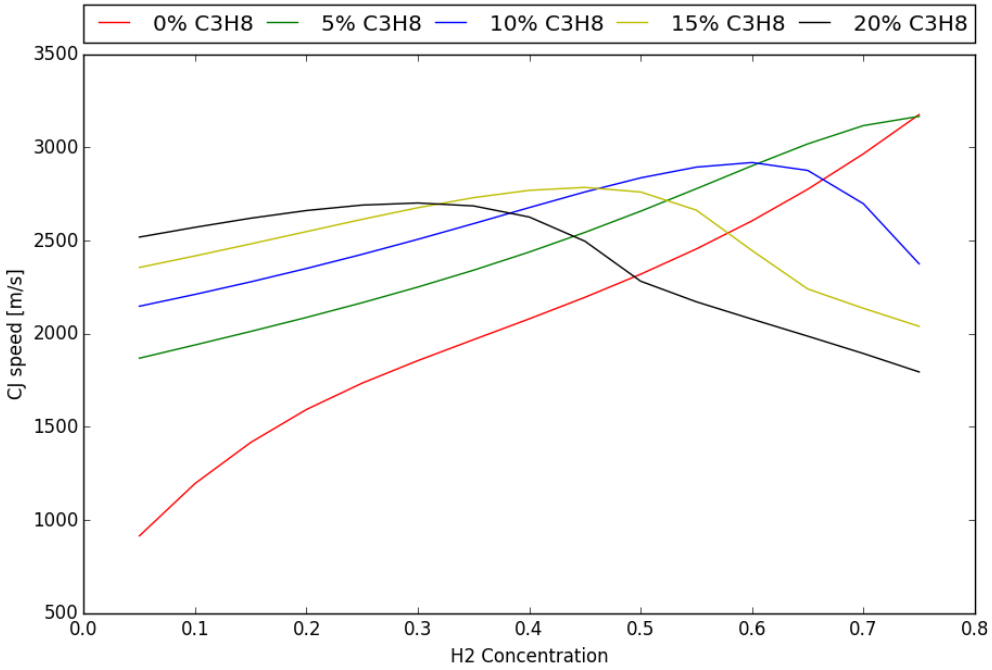

Figure 1: . Chapman Jouguet velocity vs H2 and C3H8 concentration

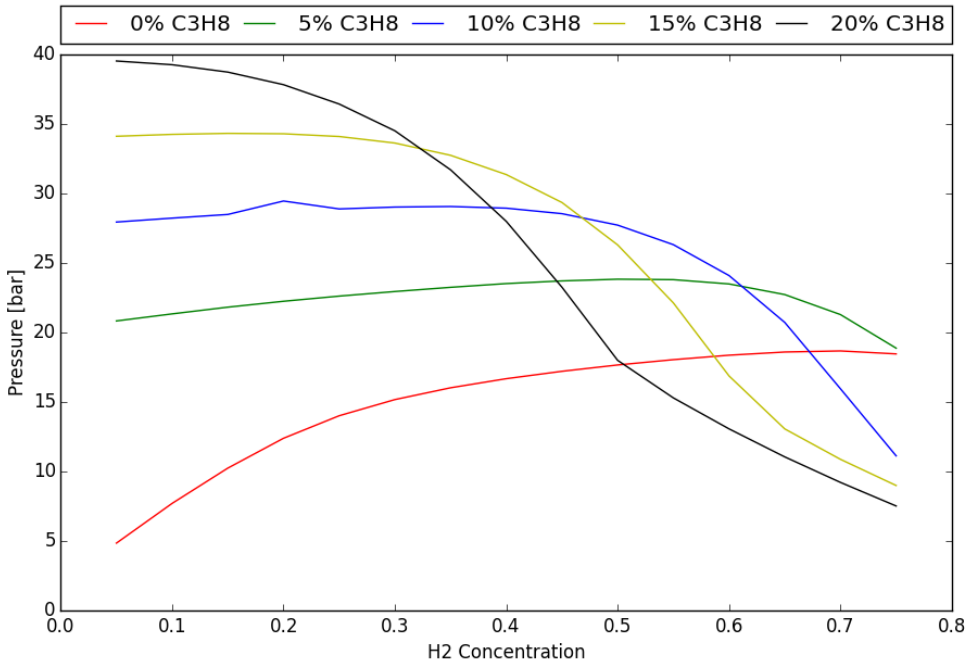

Figure 2: . Chapman Jouguet pressure vs H2 and C3H8 concentration

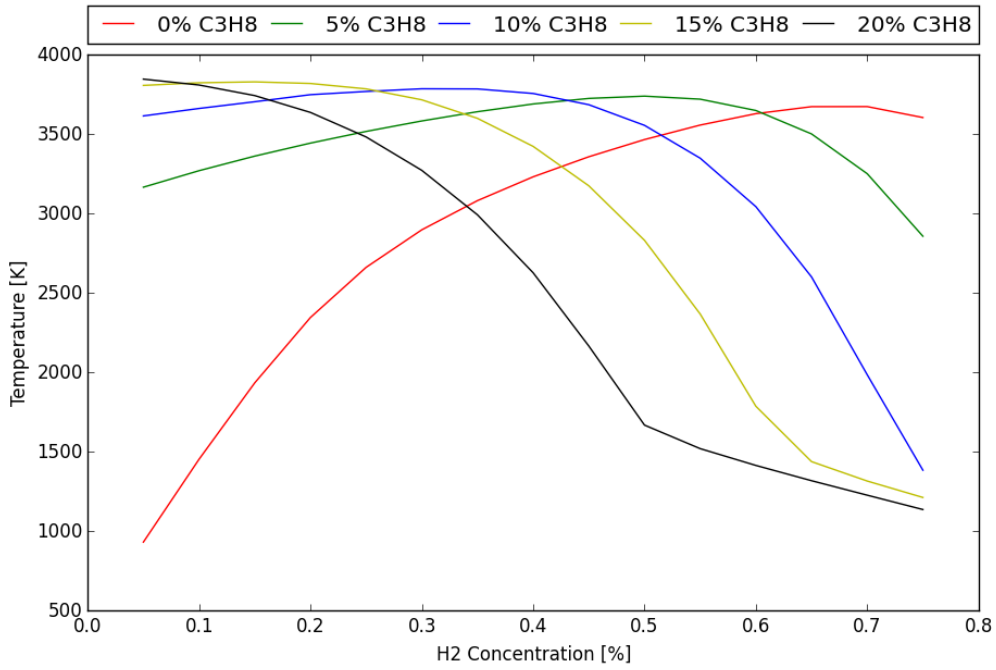

Figure 3: . Chapman Jouguet temperature vs H2 and C3H8 concentration

What can be read from Fig 1 is that there is no maximum CJ speed for a pure hydrogen - oxygen mixture. As the amount of propane increases, the point of maximum moves to the lower hydrogen concentrations. What's more, the maximum pressures are achieved for low hydrogen - high propane mixtures and the maximum temperatures are almost the same for every mixture. The sharp breaks on the plots may denote the ignition limits.

4 Summary

- The CJ speed for pure hydrogen-oxygen mixtures increases with hydrogen concentration
- With propane added, the maximum starts to appear
- Propane addition raises the maximum pressure significantly, but does not affect maximum temperature

5 References

[1] Kordylewski Wlodzimierz, Spalanie i paliwa, Oficyna Wydawnicza Politechniki Wroclawskiej, 2005