Warsaw University of Technology | Faculty of Power and Aeronautical Engineering

course
COMPUTATIONAL METHODS IN COMBUSTION

DETONATION SIMULATION OF PROPANE-AIR MIXTURE

Cantera Project

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1. Introduction

The aim of this project was to simulate the Chapman-Jouguet detonation of propane-air mixture for different concentrations and: first for constant initial pressure $p = 1bar$ and different initial temperatures, then for constant initial temperature $T = 298K$ and different initial pressures. All calculations have been done using SDToolbox and Cantera packages in Python. The results are diagrams of basic detonation parameters.

2. Model description

The simplest theory to predict the behaviour of detonation in gases is Chapman-Jouguet theory. It models the detonation as a propagating shock wave accompanied by exothermic heat release. C-J theory can be described by a set of algebraic equations called Rankine-Hugoniot equations:

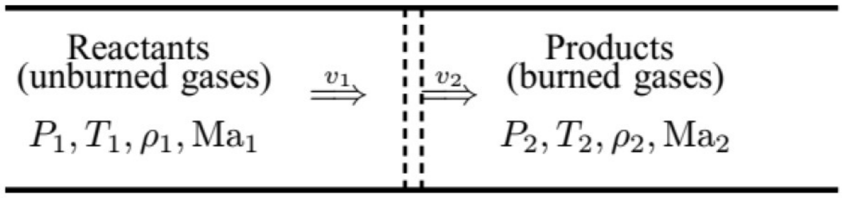

Figure 2.1. One dimensional wave propagation

$$\dot{m} = \rho_1 u_1 = \rho_2 u_2 \tag{1}$$

$$P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2 \tag{2}$$

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2} \tag{3}$$

C-J detonation is a thermodynamic parameter which depends only on mixture's initial parameters. The release of energy occurs in infinitely short period of time. The speed at which the reacting gas reaches the speed of sound relative to a datum associated with the leading shock wave is called the C-J speed:

$$U_D = \frac{\rho_2}{\rho_1} a_2 > a_1 \tag{4}$$

3. Results

The results of this simulation are diagrams showing relationships between initial pressures/temperatures and C-J speeds, post shock pressures and temperatures.

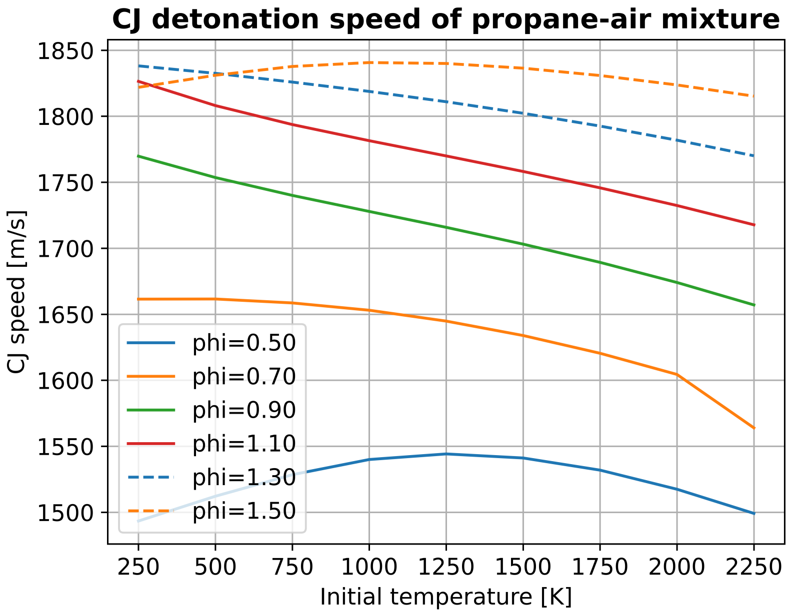

Figure 3.1. Relationship between C-J speed and initial temperature

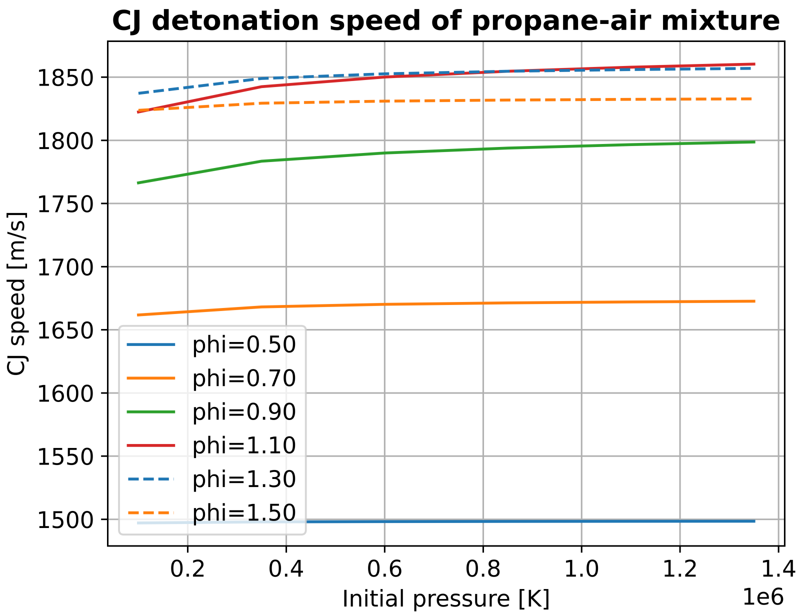

Figure 3.2. Relationship between C-J speed and initial pressure

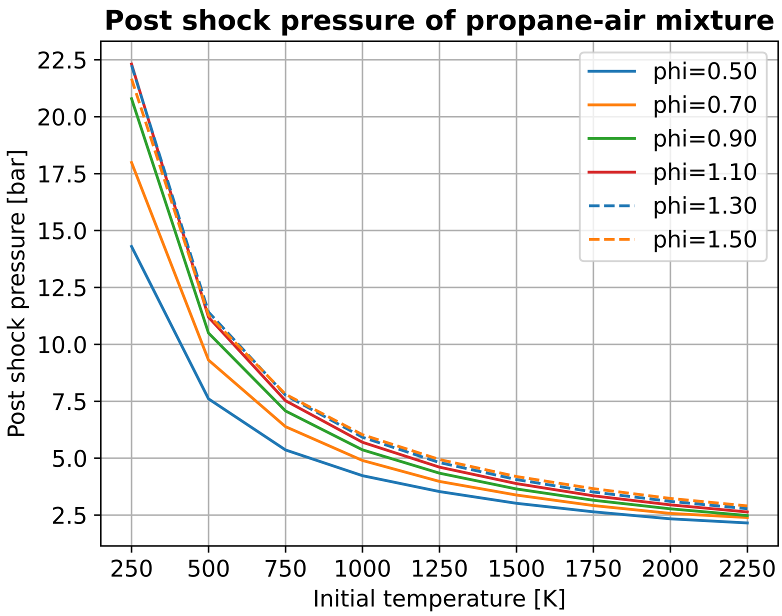

Figure 3.3. Relationship between post shock pressure and initial temperature

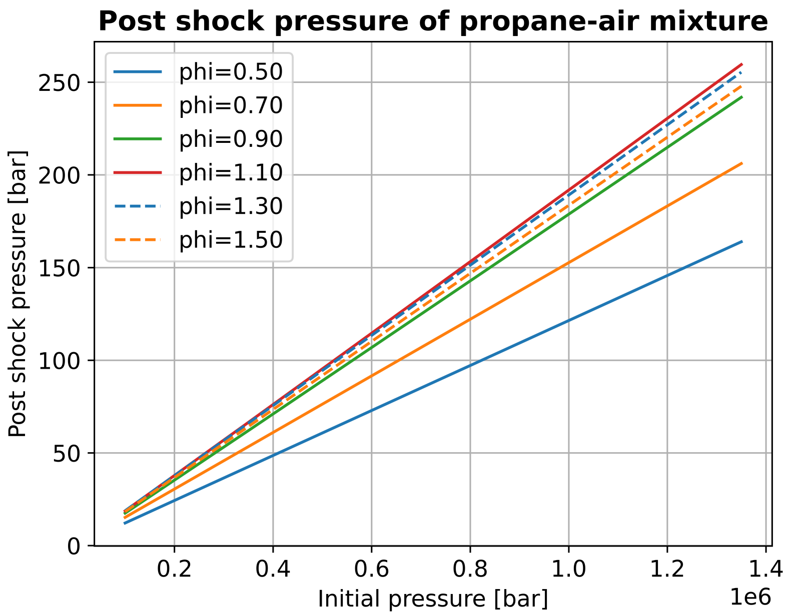

Figure 3.4. Relationship between post shock pressure and initial pressure

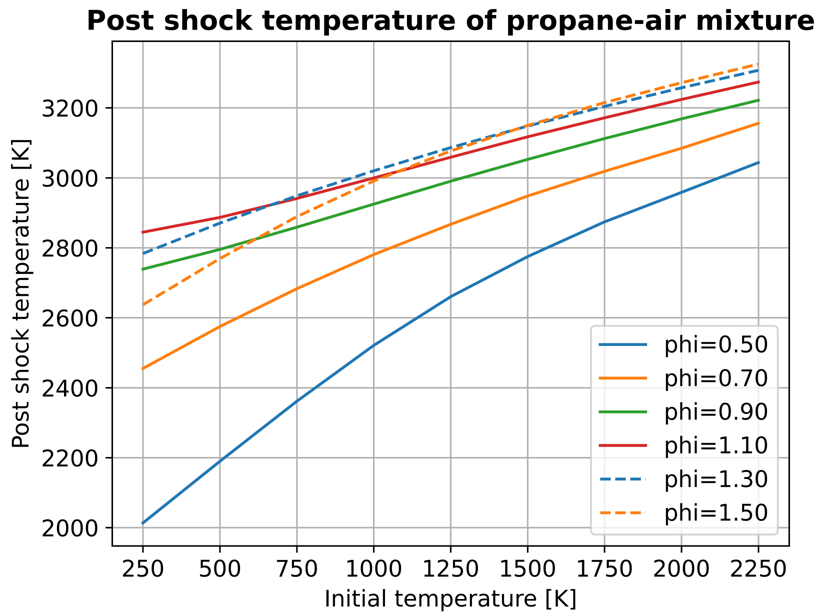

Figure 3.5. Relationship between post shock temperature and initial temperature

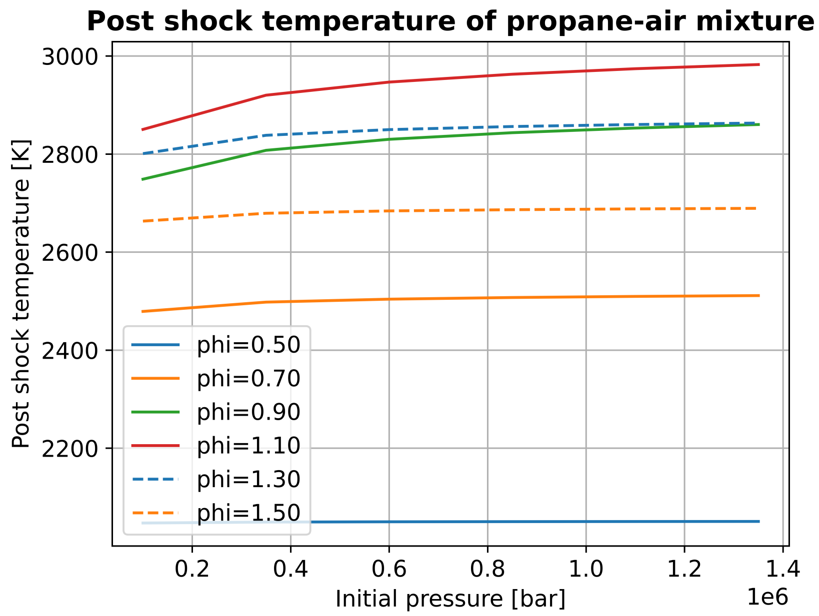

Figure 3.6. Relationship between post shock temperature and initial pressure

4. Conclusions

There are several conclusions as it can be seen on the diagrams:

1) Initial pressure does not affect C-J speed as much as initial temperature.
2) C-J speed decreases as initial temperature increases.
3) Post shock pressure increases as initial pressure increases and decreases as initial temperature increases.
4) Post shock temperature is almost constant the higher the initial pressure is and increases the higher the initial temperature is.

Bibliography

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