Warsaw University of Technology
The Faculty of Power and Aeronautical Engineering

Computational Methods in Combustion

Detonation parameters of hydrogen-air, ethane-air, ethyl-air, methane-air, propane-air and propyl-air mixtures for different initial values of pressure and temeratures

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Contents

1 Introduction

Aim of this report is to show different parameters of detonation for various compositions of hydrogen-air, ethane-air, ethyl-air, methane-air, propane-air and propyl-air mixtures. For different initial values of temperature and pressure there were calculated pressure, temperature and velocity of detonation. To calculate these parameters SDToolbox and Cantera were used.

2 Method description

In order to calculate certain parameters of detonation it is necessary to compute CJ-speed. Using SDToolbox package for Cantera it is possible to calculate CJ-speed with "CJspeed" command. For every initial state and composition of gas mixtures it returns CJ-speed. By "PostShock.eq" command it is possible to obtain pressure and temperature of detonation. "PostShock.eq" command uses initial values of pressure, temperature and previously computed CJ-speed for a given case, then returns post-shock values of pressure and temperature. Gas models were taken from "gri30.cti.

3 Review of the literature

1. N. S. Astapov, Yu. A. Nikolaev, V. Yu. Ul'yanitski
"Detonation parameters of hydrogen–oxygen and hydrogen–air mixtures at high initial density"
In this study the authors measured detonation parameters for initial values of pressure at 0,1-1000 atm and temperatures at 80-1000 K, for hydrogen-air mixtures. Parameters were calculeted for nonideal gas described by a Van der Waals equation of state. Research show that using ideal gas model is inappropriate for pressure larger than 10 atm for detonation. Differences between calculations for ideal and nonideal gas were about 1 percent at p=10 atm and 7-12 percent at p=100 atm.

2. R.K. Zipf Jr., V.N. Gamezo, M.J. Sapko, W.P. Marchewka, K.M. Mohamed, E.S. Oran, D.A. Kessler,E.S. Weiss, J.D. Addis, F.A. Karnack, D.D. Sellers
"Methaneeair detonation experiments at NIOSH Lake Lynn Laboratory"
This article was based on experiments made using explosion tube for methane-air mixtures. Results form experiment were compared to computed CJ detonation. Both results agreed to within experimental error of associated with this pressure measurement inside detonation tube.

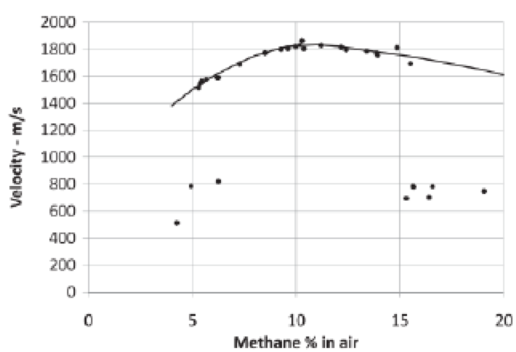

Figure 1: Measured detonation velocity (data points) and CJ detonation velocity (solid line) versus methane in air.

3. V. Yu. Gidaspov and N. S. Severina
"Numerical Simulation of the Detonation of a Propane-Air Mixture, Taking Irreversible Chemical Reactions into Account"
In this publication numerical methods were used based on integral laws of mass, pulse, and energy conservation for propane-air mixtures. This study was mainly aimed at deciding whether applying kinetic mechanisms

with irreversible chemical reactions for describing detonation of propane in air is appropriate. Researchers came into conclusion that it is acceptable when time of passing of the system to equilibrium state exceeds time of research interest.

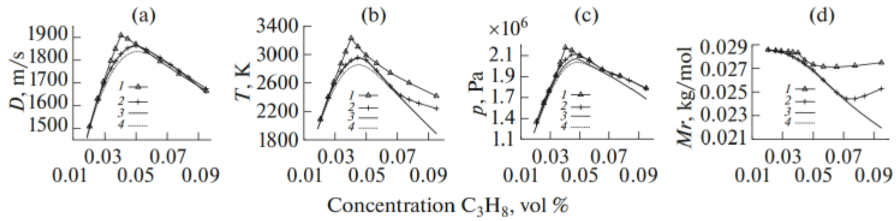

Figure 2: Distribution of mixture parameters depending on mole fraction of propane for initial pressure p0 = 101325 Pa: 1 − irreversible chemical reactions; 2 − reversible chemical reactions; 3, 4 − equilibrium computation of 7 and 18 substances, respectively.

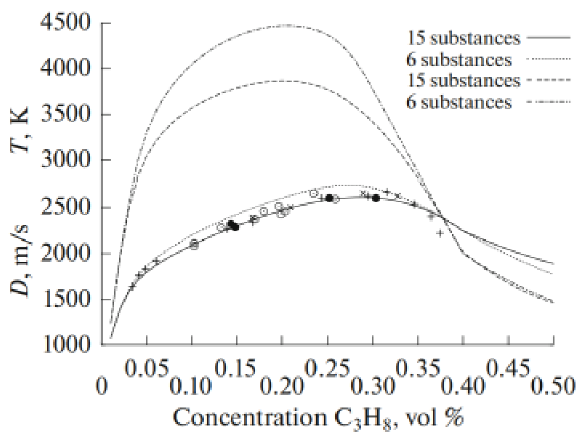

Figure 3: Computed dependencies of Chapman-Jouguet detonation velocity (two lower curves) and temperature (two upper curves) on mole fraction of 38; markers—experimental data [10] (p0 = 101325 Pa, T0= 293.15 K).

4 Results

Results are calculated for: a) constant temperature T=295 K, when presented for different pressure b) constant pressure p=1 bar, when presented for different temperatures

4.1 Hydrogen-air

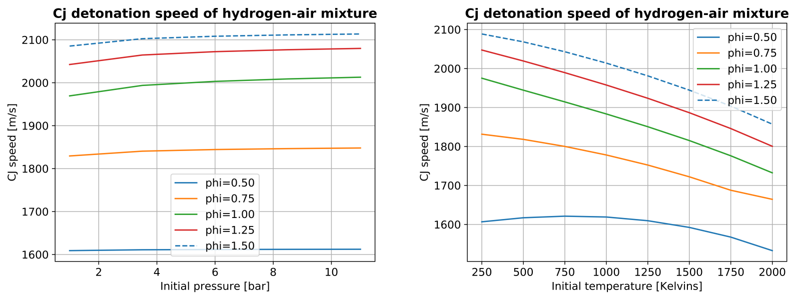

Figure 4: The relationship between CJ speed and initial pressure or temperature

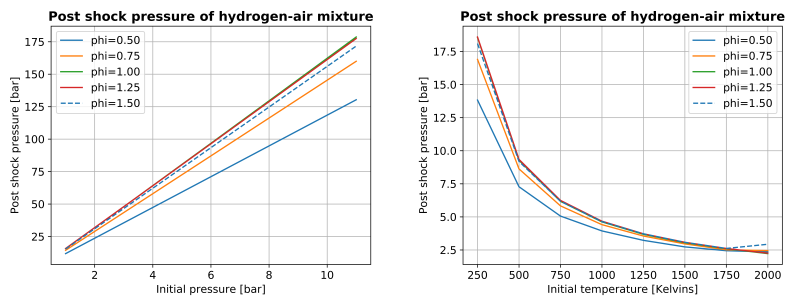

Figure 5: The relationship between post shock pressure and initial pressure or temperature

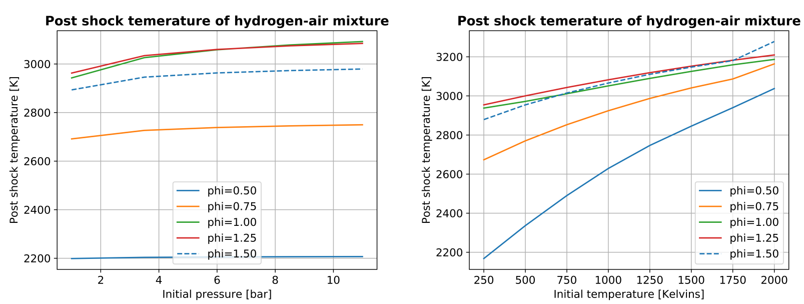

Figure 6: The relationship between post shock temperature and initial pressure or temperature

4.2 Ethane-air

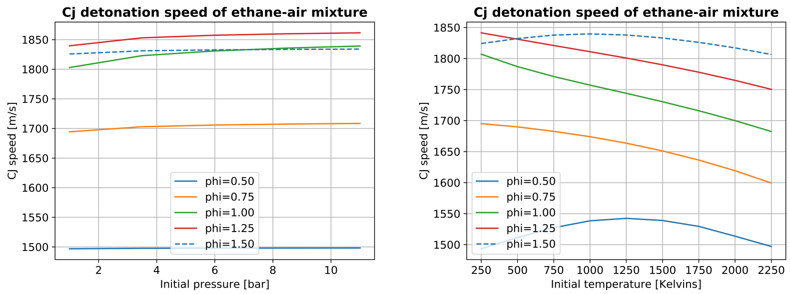

Figure 1: The relationship between CJ speed and initial pressure or temperature

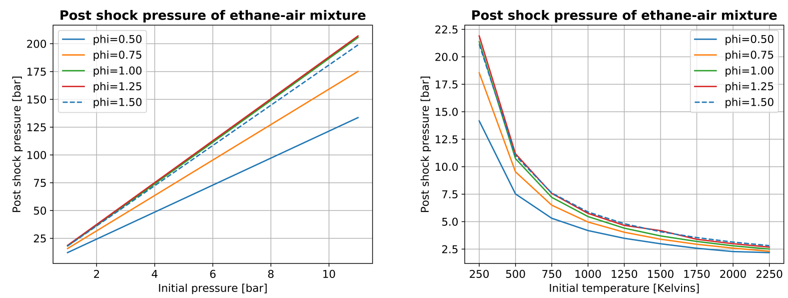

Figure 2: The relationship between post shock pressure and initial pressure or temperature

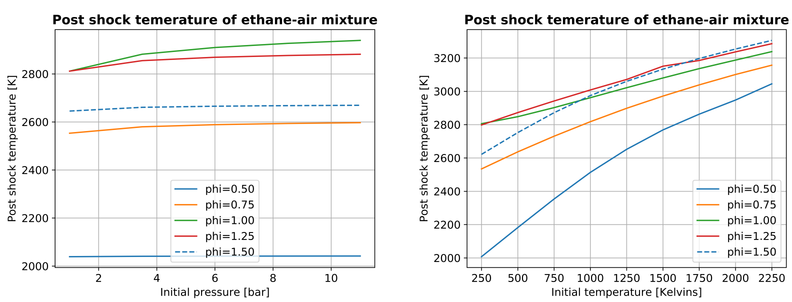

Figure 3: The relationship between post shock temperature and initial pressure or temperature

4.3 Ethyl-air

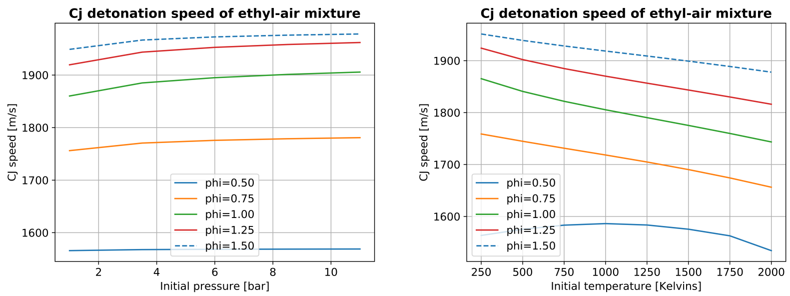

Figure 1: The relationship between CJ speed and initial pressure or temperature

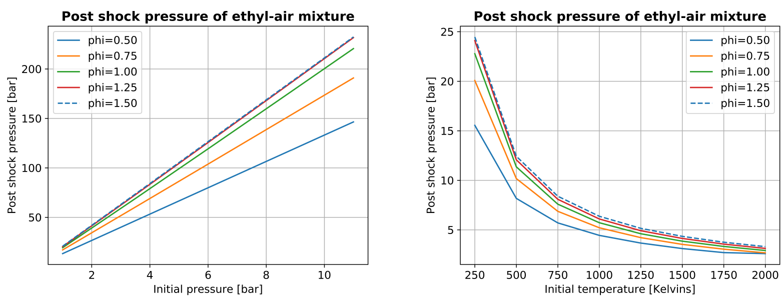

Figure 2: The relationship between post shock pressure and initial pressure or temperature

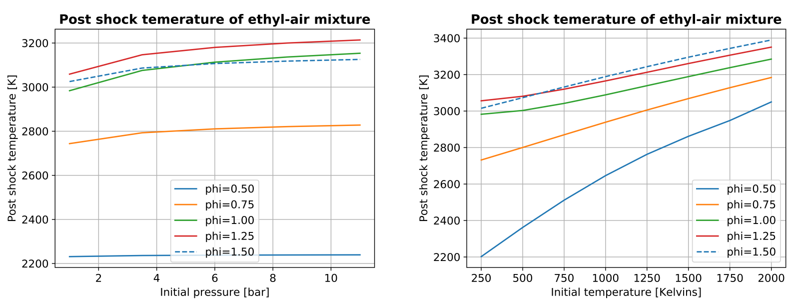

Figure 3: The relationship between post shock temperature and initial pressure or temperature

4.4 Methane-air

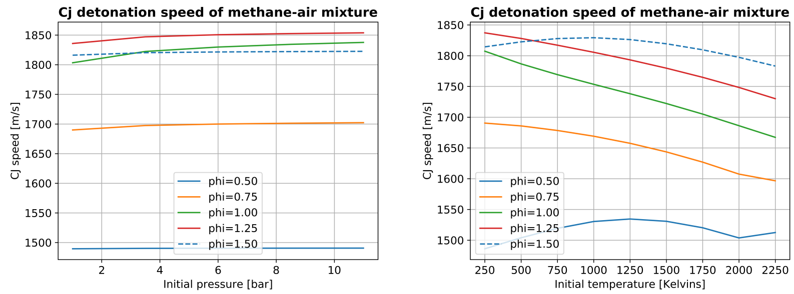

Figure 1: The relationship between CJ speed and initial pressure or temperature

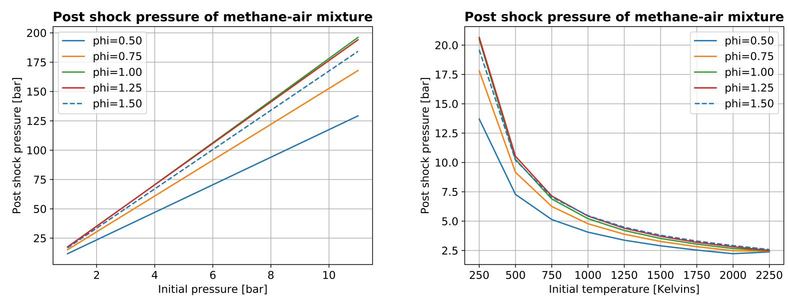

Figure 2: The relationship between post shock pressure and initial pressure or temperature

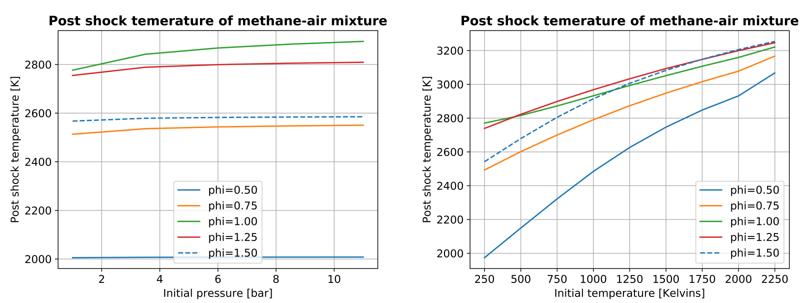

Figure 3: The relationship between post shock temperature and initial pressure or temperature

4.5 Propane-air

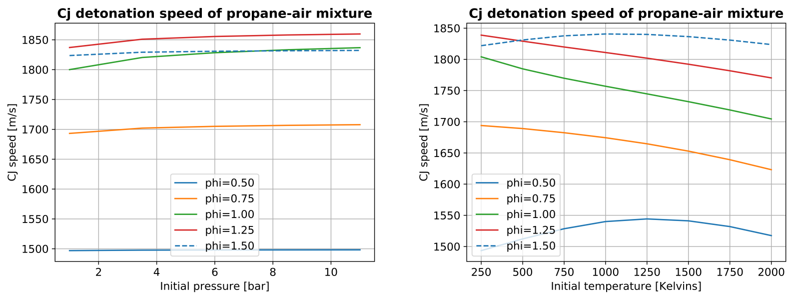

Figure 1: The relationship between CJ speed and initial pressure or temperature

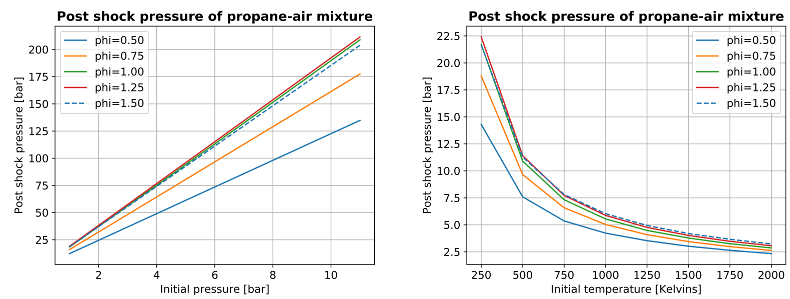

Figure 2: The relationship between post shock pressure and initial pressure or temperature

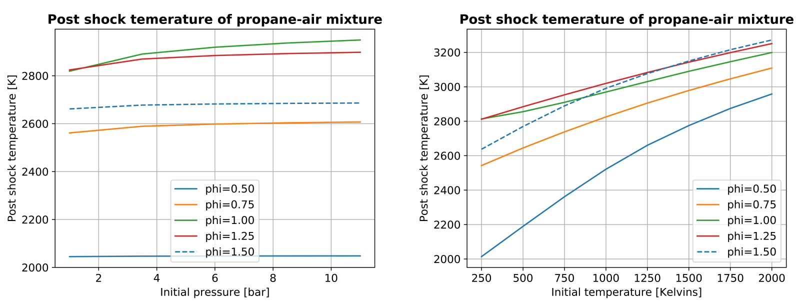

Figure 3: The relationship between post shock temperature and initial pressure or temperature

4.6 Propyl-air

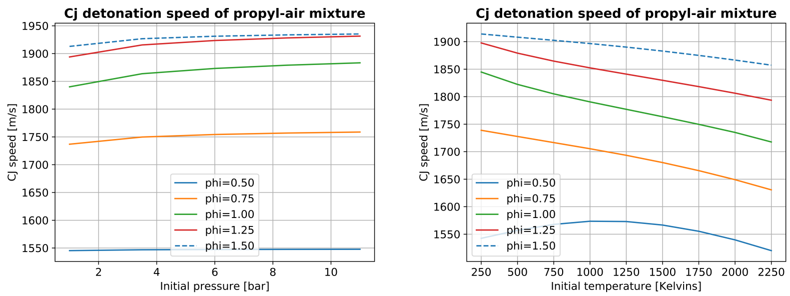

Figure 1: The relationship between CJ speed and initial pressure or temperature

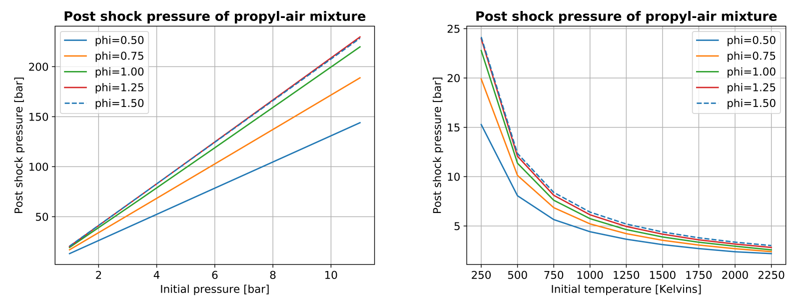

Figure 2: The relationship between post shock pressure and initial pressure or temperature

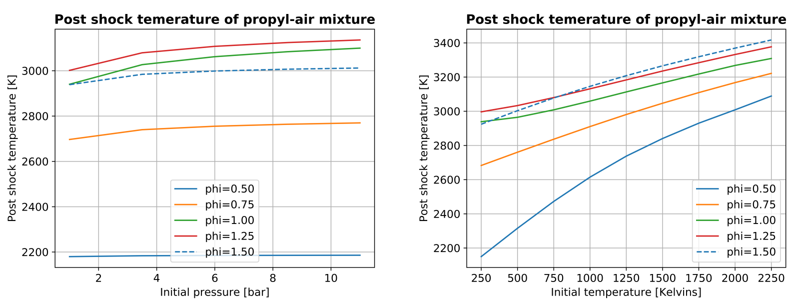

Figure 3: The relationship between post shock temperature and initial pressure or temperature

5 Conclusions

As it is visible on the plots:
a) initial pressure does not affect significantly CJ speed and post shock temperature
b) CJ speed decreases the higher the initial temperature is
c) post shock temperature increases the higher the initial temperature is
d) post shock pressure significantly lower when initial temperature is higher
e) post shock pressure increases linearly when we increase initial pressure.

References

[1] **N. S. Astapov, Yu. A. Nikolaev, V. Yu. Ul'yanitski**
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[2] **R.K. Zipf Jr., V.N. Gamezo, M.J. Sapko, W.P. Marchewka, K.M. Mohamed, E.S. Oran, D.A. Kessler,E.S. Weiss, J.D. Addis, F.A. Karnack, D.D. Sellers**
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[3] **V. Yu. Gidaspov and N. S. Severina**
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