Metody Komputerowe w Spalaniu

Ignition delay for hydrogen and alkane mixtures with air

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Contents

1 Introduction

In the report below there are presented analisys of the impact of the starting conditions on the ignition delay time. Calculations were performed for four types of mixtures: hydrogen - air, methane - air, ethane - air and propane - air. There were used different starting values of temperature, pressure and equivalence ratio.

2 Description of the method

2.1 Calculation method

Calculations for every case were made using GRI-Mech 3.0 reaction mechanism in Cantera package for Python. The ignition delay time shows how much time mixture needs to ignite under specific conditions. To obtain this value for mixtures mentioned above constant volume of reactor was established.

2.2 Initial conditions

As a initial conditions was assumed temperature equals $T = 1000K$ and pressure $P = 1bar$.

Equestions of combustion on which calculations were based (stechiometric mixture):

Hydrogen

$$2H_2 + O_2 + 3,76N_2 \rightarrow 2H_2O + 3,76N_2 \tag{2.1}$$

Methane

$$CH_4 + 2(O_2 + 3,76N_2) \rightarrow CO_2 + 2H_2O + 7,52N_2 \tag{2.2}$$

Ethane

$$C_2H_6 + 3,5(O_2 + 3,76N_2) \rightarrow 2CO_2 + 3H_2O + 13,16N_2 \tag{2.3}$$

Propane

$$C_3H_8 + 5(O_2 + 3,76N_2) \rightarrow 3CO_2 + 4H_2O + 18,8N_2 \tag{2.4}$$

2.3 Ignition delay visualisation

Visualisation of the ignition delay is shown below (Figure 2.1).

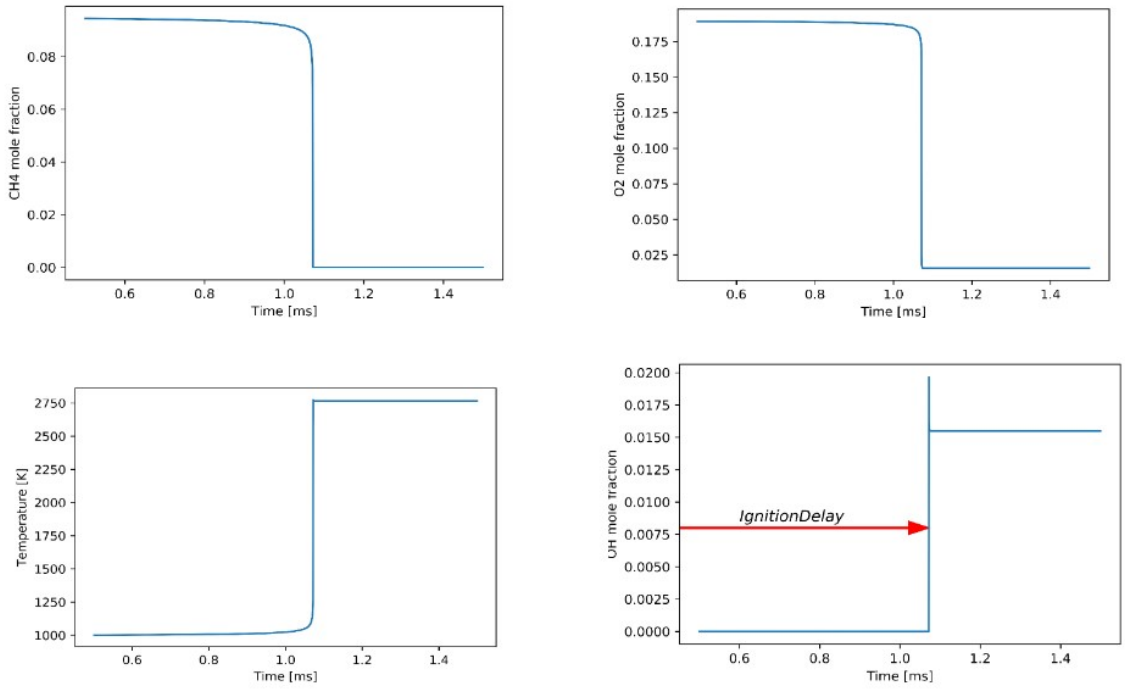

Figure 2.1: Change of parameters over time for methane - air mixture (with visible ignition time)

In a specific moment mole fraction of fuel and oxygen, but also OH decreases rapidly. This point can be defined as a start of the ignition. The time interval between the start of the simulation and the start of the ignition is the ignition delay. As a result it may be calculated from occurence of the OH species concentration peak. The programme used in this project is based on this statement.

3 Literature

In study [2] were performed experiments with hydrogene - air mixture with electrostatic ignition. Also the time evolutions of the OH density and the gas temperature are measured after ignition.

In [3] study authors measured ignition delay of methane - air mixture using shock tube method to evaluate the commonly used kinetic models. Calculations were performed for three of them: GRI Mech 3.0, USC Mech II, Aramco Mech 1.3. Experimental results were compared with computed values. In addition authors decided which kinetics models are the most accurate at specific conditions. They concluded that GRI Mech 3.0 model, used in this report, underpredicts the ignition delay for high pressures and overpredicts them for rich mixtures.

Similarly to numerous different publications, article [5] compares experimental and calculated values of ignition delay of propane - hydrogen mixture. Authors used experimental data from earlier studies. Simulations were performed using two kinetics models: NUI Mech and USC Mech II.

4 Results

For all of the types of mixtures were visualised two kinds of plots:

- the relationship between ignition delay and initial temperature (for constant pressure and several values of exuivalence ratio),
- the relationship between ignition delay and initial pressure (for constant temperature and several values of exuivalence ratio).

4.1 Hydrogen

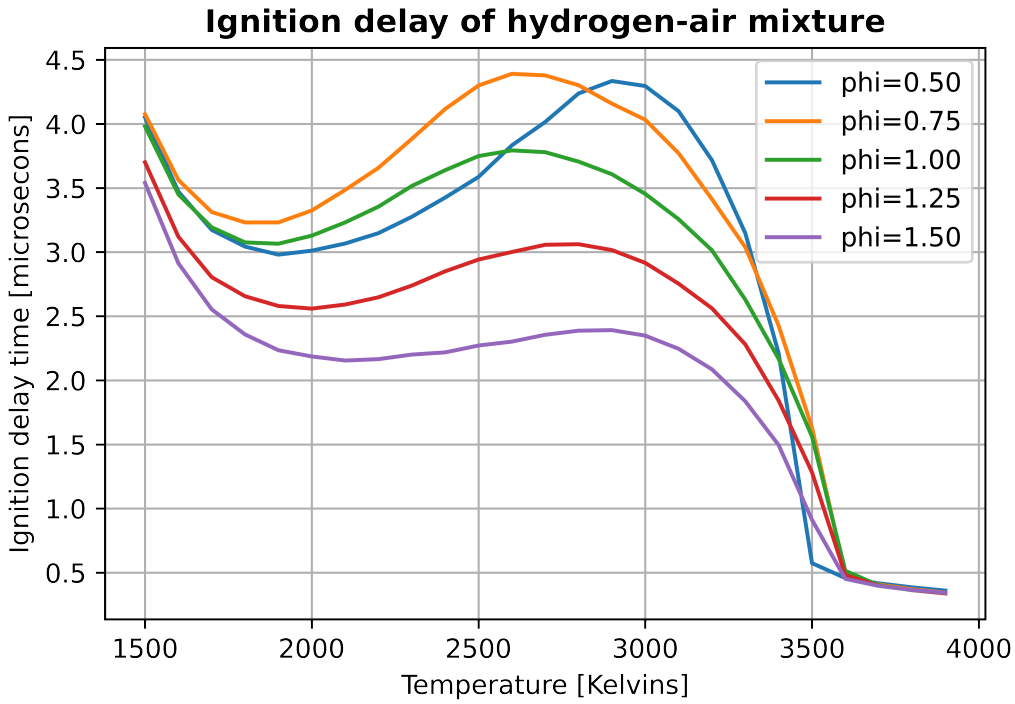

Figure 4.1: Ignition delay as a function of the temperature for hydrogen - air mixture

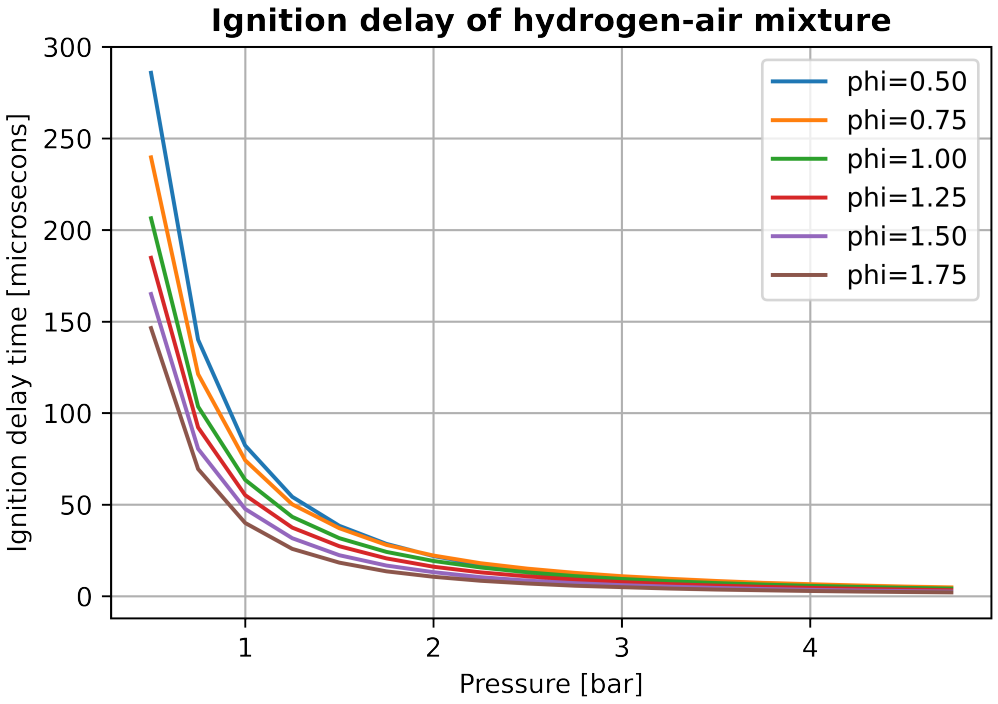

Figure 4.2: Ignition delay as a function of the pressure for hydrogen - air mixture

4.2 Methane

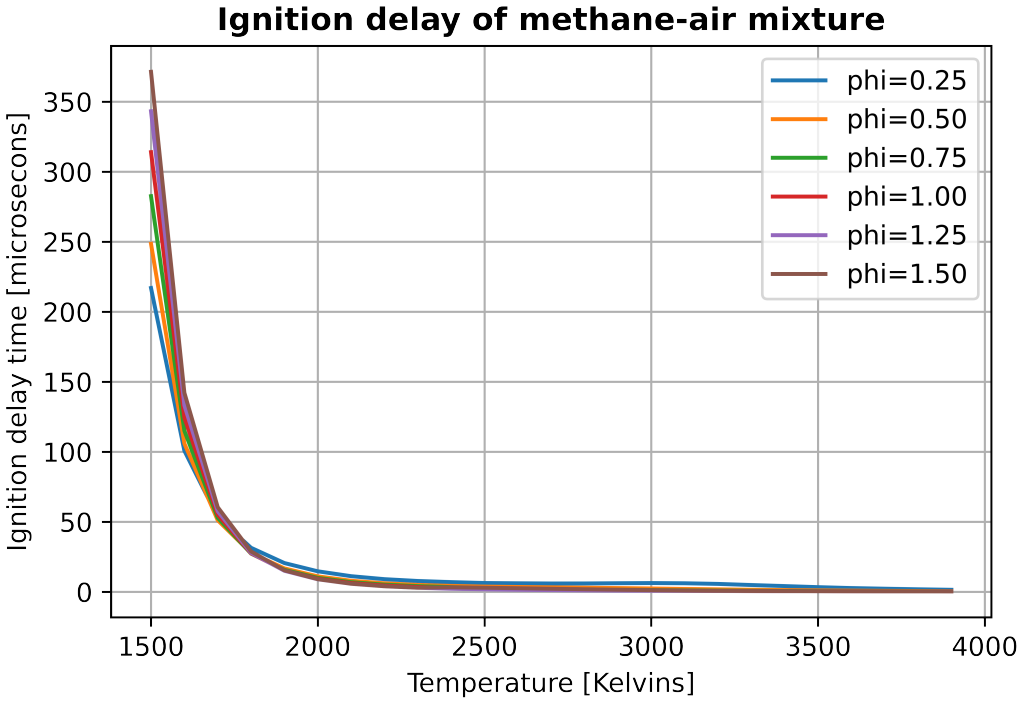

Figure 4.3: Ignition delay as a function of the temperature for methane - air mixture

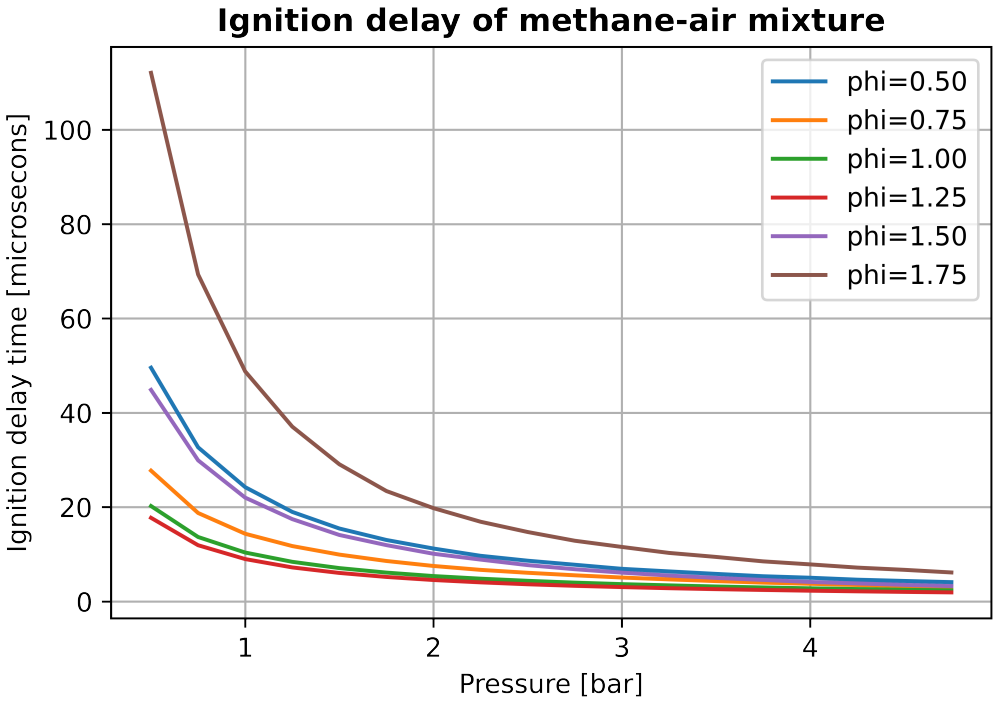

Figure 4.4: Ignition delay as a function of the pressure for methane - air mixture

4.3 Ethane

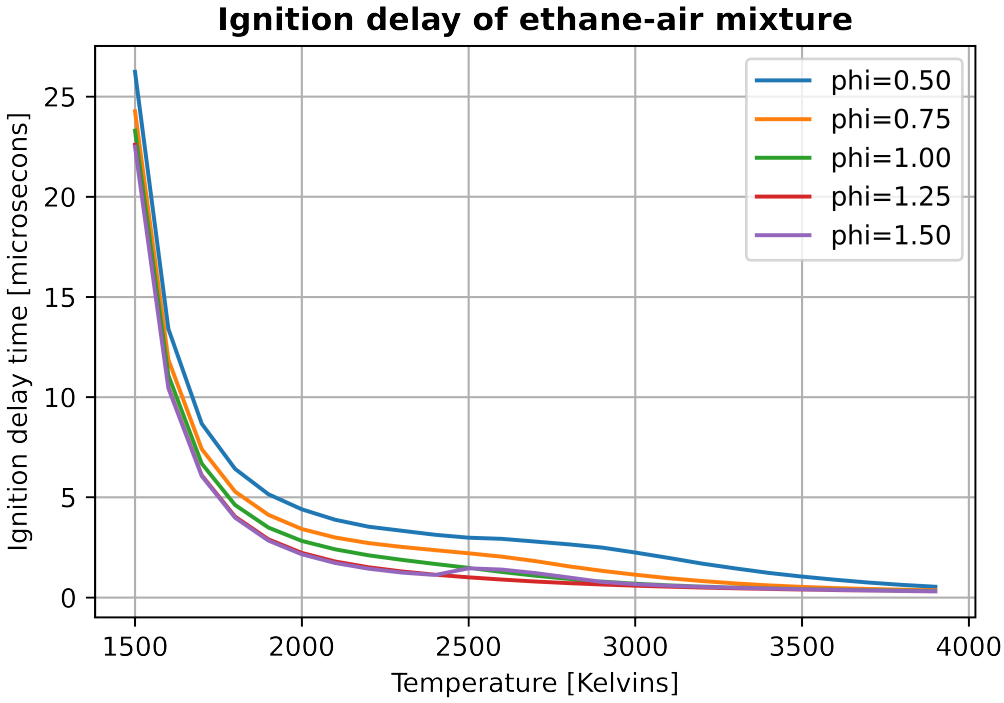

Figure 4.5: Ignition delay as a function of the temperature for ethane - air mixture

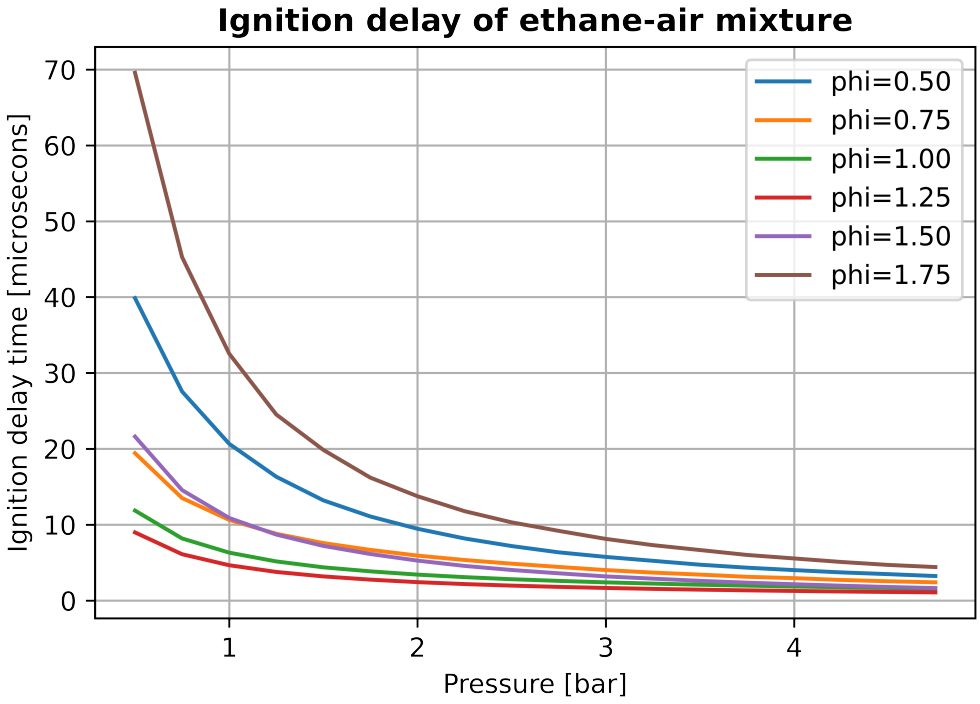

Figure 4.6: Ignition delay as a function of the pressure for ethane - air mixture

4.4 Propane

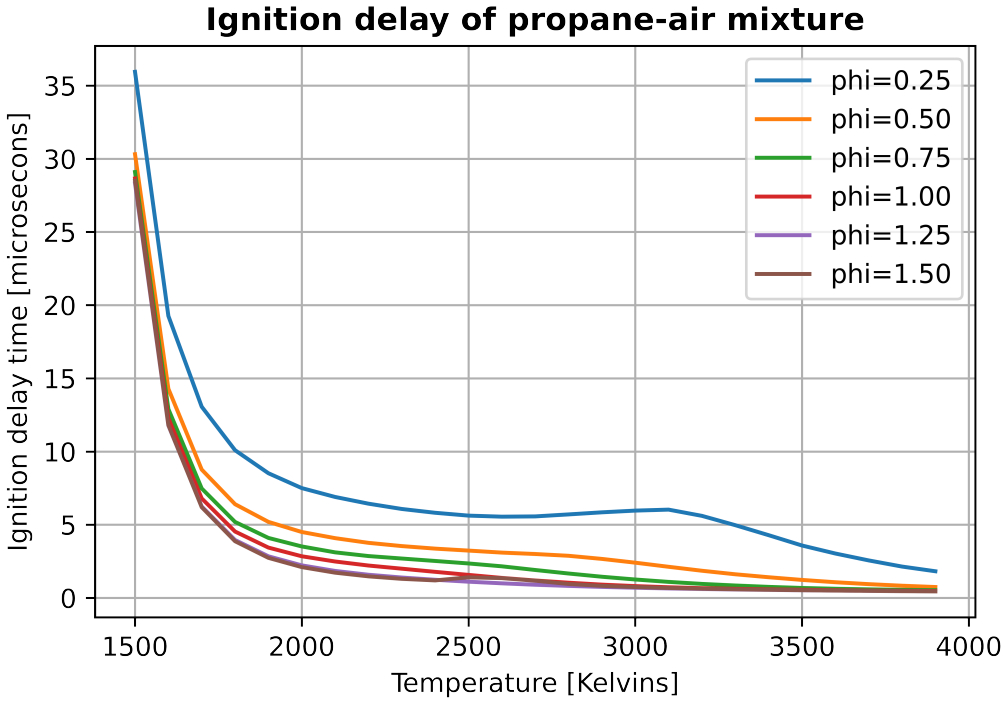

Figure 4.7: Ignition delay as a function of the temperature for propane - air mixture

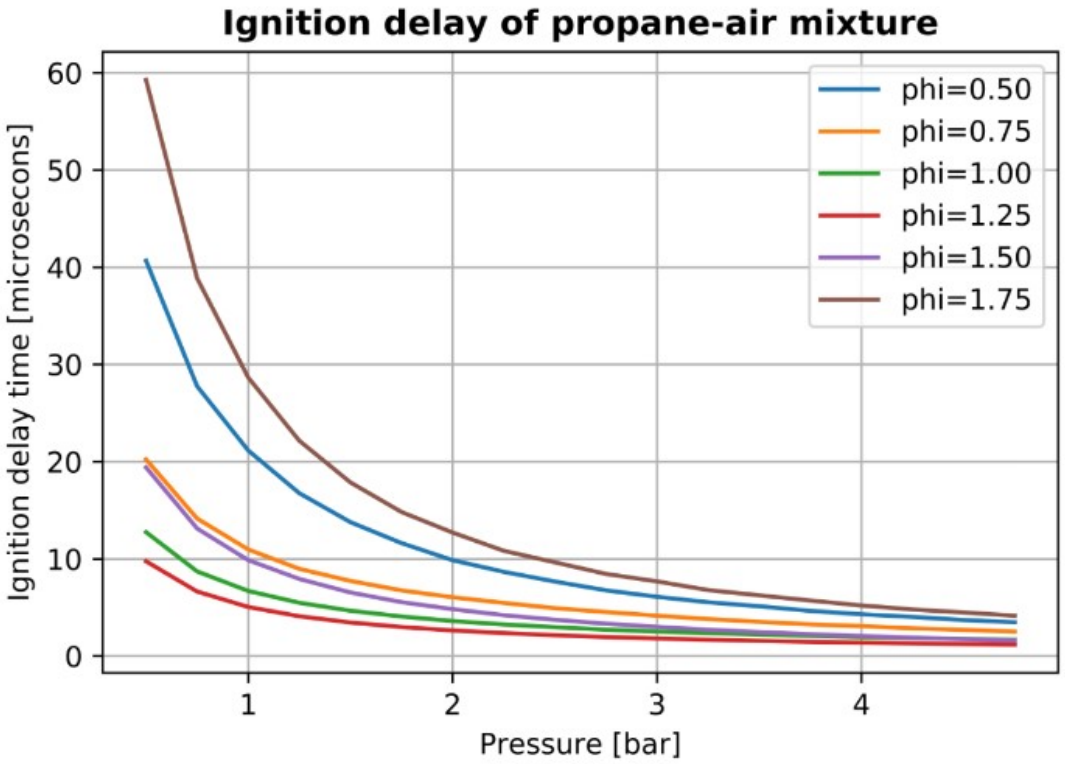

Figure 4.8: Ignition delay as a function of the pressure for propane - air mixture

5 Conclusions

The ignition delay depends on the initial temperature, pressure and equivalence ratio. As it is shown on the plots, in most cases the ignition delay significantly decreases with the growth ot the temperature or pressure. The one exeption is hydrogen - air mixture with constant pressure and changing temperature. The curves take characteristic shape - the maximum point of the ignitiion value states between 2500 and 3000 K.

It can also be noticed, that for wide range of initial conditions the ignition delay is the shortest around stoichiometry, for a little rich mixture. In the cases of the very poor or very rich compositions mixture is hard to ignite. It is easy to see that high temperatures and pressures with stoichiometry are the better conditions to quick igniton.

Values calculated in this project are very similat to experimental data [3].

6 Bibliography

[1] https://github.com/Rorjh/MKWS1

[2] Ryo Ono, Tetsuji Oda *Spark ignition of hydrogen - air mixture*, Journal of Physics, 2008

[3] Erijang Hu, Xiaotian Li, Xin Mend, Yizhen Chen, Yu Cheng, Yongliang Xie, Zuohua Huang *Laminar flame speeds and ignition delay times of methane - air mixtures at elevated temperatures and pressures*, Xi'an Jiaotong Univeristy, 2015

[4]Erijang Hu, Yizhen Chen, Zhang Zihang, Ii Xiaotian *Experimental Study on Ethane Ignition Delay Times and Evaluation of Chemical Kinetic Models*, Xi'an Jiaotong Univeristy, 2015

[5] Xingjia Man, Chenglong Tang, Liangjie Wei, Lun Pan, Zuohua Huang *Measurements and kinetic study on ignition delay times of propane/hydrogen in argon diluted oxygen*, Xi'an Jiaotong Univeristy, 2013

[6] Zhao ZhenLong, Chen Zheng, Chen ShiYi *Correlations for the ignition delay times of hydrogen/air mixtures*, Peking Univeristy, 2010

List of Figures