Politechnika Warszawska

Computational Methods in Combustion

Ignition delay for alkane, alkene and alkyne mixtures with air

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1 Introduction

Below is presented an analysis of the influence of initial conditions on ignition delay time. Calculations were conducted for four different mixtures: methane with air, ethane with air, ethylene with air and acetylene with air. The research considered varied initial values of temperature, pressure, and equivalence ratio.

2 Description of the method

2.1 Calculation method

For each scenario, the calculations were performed using the GRI-Mech 3.0 reaction mechanism within the Cantera package for Python. The ignition delay time indicates the duration required for a mixture to ignite under specific circumstances. To determine this value for the aforementioned mixtures, a reactor with a fixed volume was employed.

2.2 Initial conditions

As an initial conditions was assumed temperature equals $T = 2000K$ and pressure $P = 5bar$.

Equations of combustion on which calculations were based (stoichiometric mixture):

Methane

$$CH_4 + 2(O_2 + 3,76N_2) \rightarrow CO_2 + 2H_2O + 7,52N_2 \tag{1}$$

Ethane

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

Ethylene

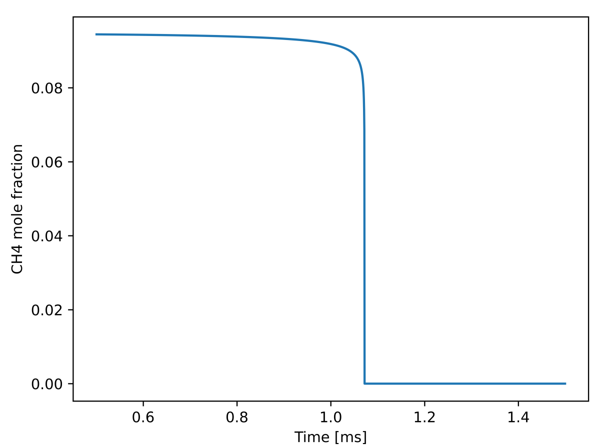
$$C_2H_4 + 3(O_2 + 3,76N_2) \rightarrow 2CO_2 + 2H_2O + 7,52N_2 \tag{3}$$

Acethylene

$$C_2H_2 + 2,5(O_2 + 3,76N_2) \rightarrow 2CO_2 + H_2O + 9,4N_2 \tag{4}$$

2.3 Ignition delay visualisation

Visualisation of the ignition delay is shown below (Figure 1).



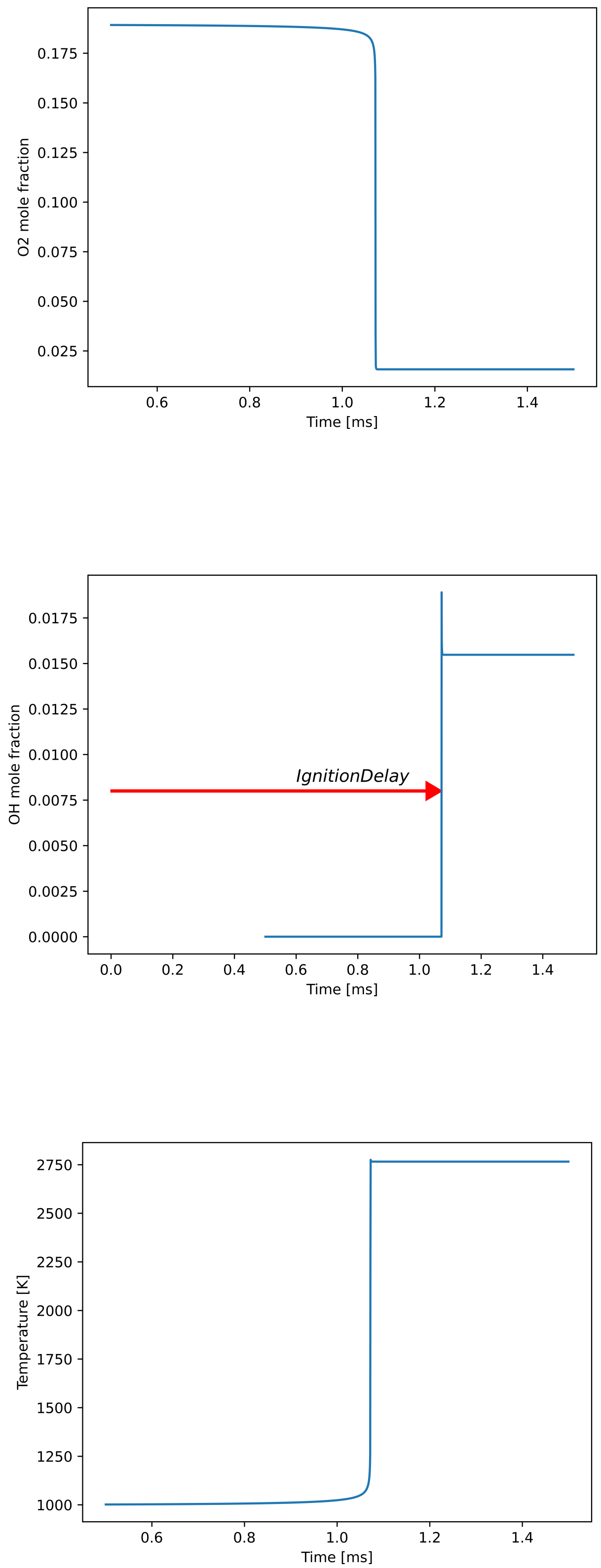


Figure 1: Change of parameters over time for methane - air mixture (with visible ignition time

At a particular instance, the concentration of fuel, oxygen, and OH species experiences a rapid decrease. This moment can be identified as the ignition initiation. The duration between the beginning of the simulation and the ignition initiation is referred to as the ignition delay. Consequently, the ignition delay can be determined by observing the peak concentration of the OH species. The software employed in this project operates based on this principle.

3 Literature

In study [2], experiments were conducted using an electrostatic ignition method with a hydrogen-air mixture. The evolution of OH density and gas temperature was measured after ignition.

In [3], the authors investigated the ignition delay of a methane-air mixture using the shock tube method to assess commonly used kinetic models. Three models, namely GRI Mech 3.0, USC Mech II, and Aramco Mech 1.3, were employed for the calculations. The experimental results were compared with the computed values. The authors determined the most accurate kinetic models under specific conditions. It was concluded that the GRI Mech 3.0 model, utilized in this report, underestimates the ignition delay for high pressures and overestimates it for rich mixtures.

Similarly to various other publications, article [5] compares the experimental and calculated ignition delay values for a propane-hydrogen mixture. The authors utilized experimental data from previous studies and performed simulations using two kinetics models: NUI Mech and USC Mech II.

4 Results

Two types of plots were generated to visualize the data for all mixture types:

- The plots depicted the correlation between ignition delay and initial temperature, considering constant pressure and various equivalence ratio values.

- The relationship between ignition delay and initial pressure was illustrated while keeping the temperature constant and using different equivalence ratio values.

4.1 Methane

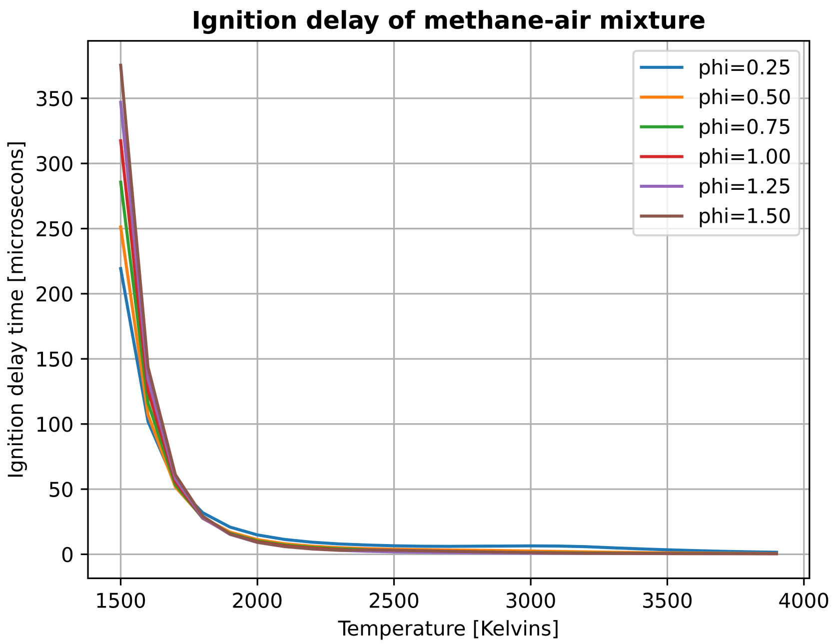


Figure 2: Ignition delay as a function of the temperature for methane - air mixture

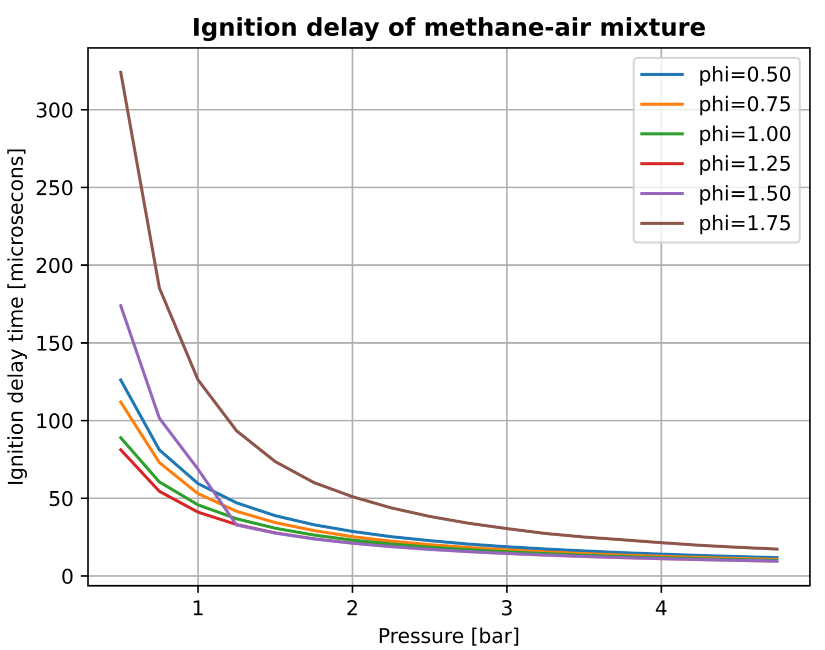


Figure 3: Ignition delay as a function of the pressure for methane - air mixture

4.2 Ethane

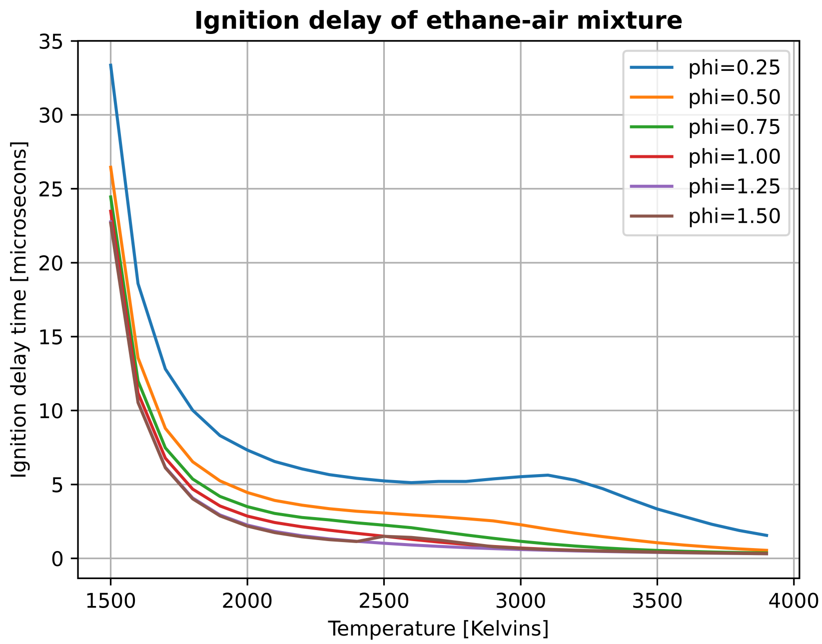


Figure 4: Ignition delay as a function of the temperature for ethane - air mixture

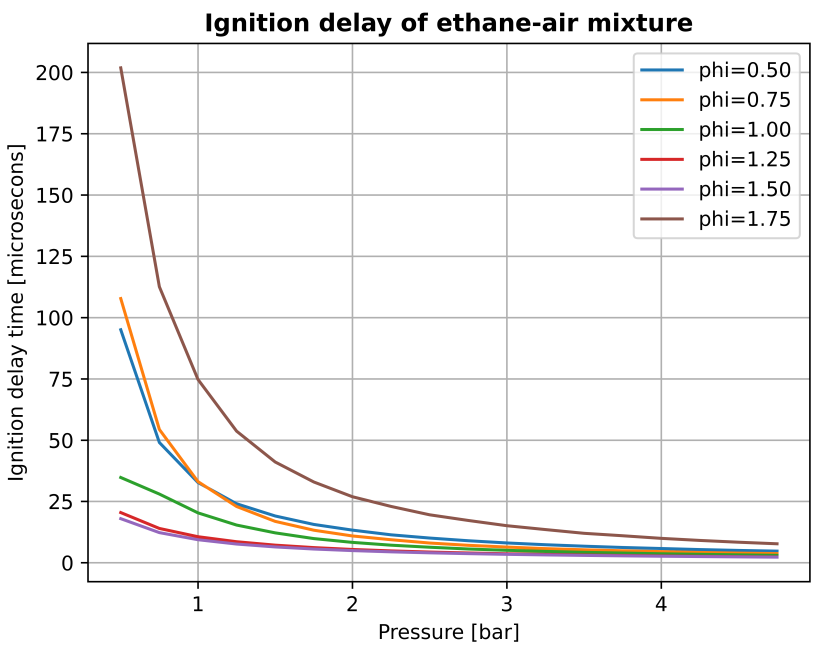


Figure 5: Ignition delay as a function of the pressure for ethane - air mixture

4.3 Ethylene

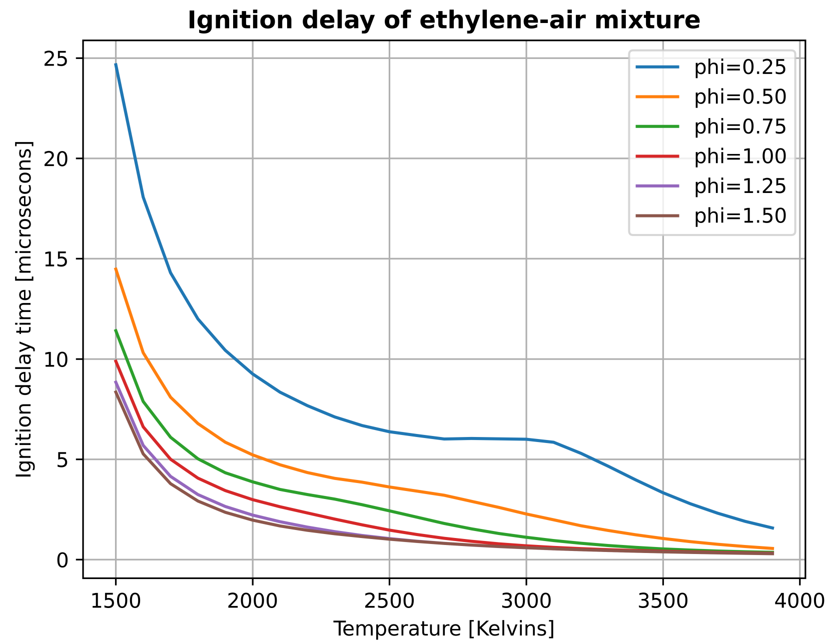


Figure 6: Ignition delay as a function of the temperature for ethylene - air mixture

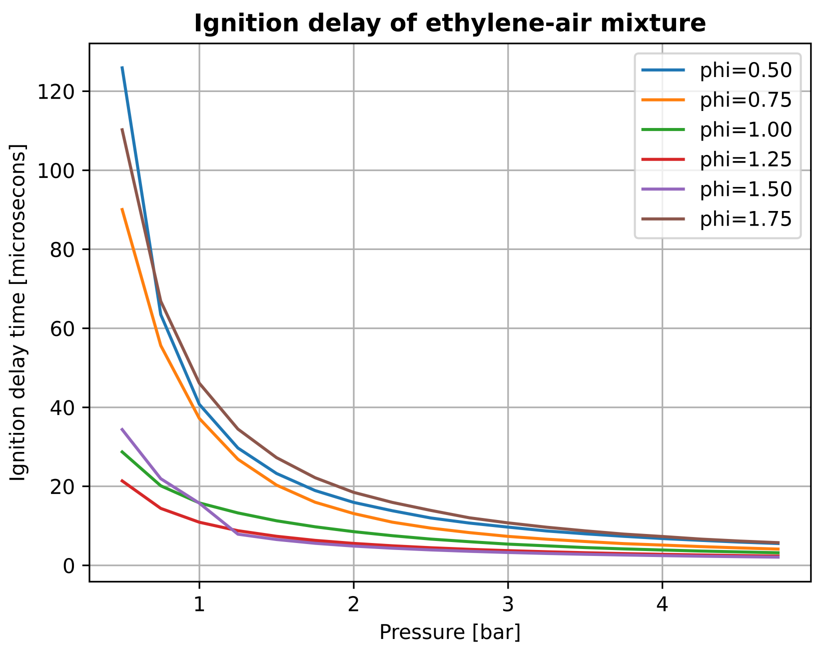


Figure 7: Ignition delay as a function of the pressure for ethylene - air mixture

4.4 Acethylene

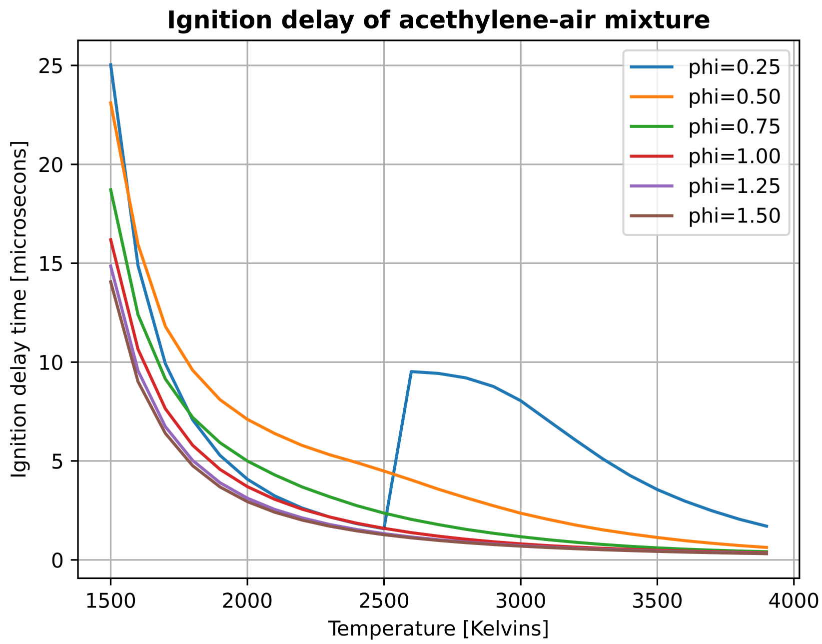


Figure 8: Ignition delay as a function of the temperature for acethylene - air mixture

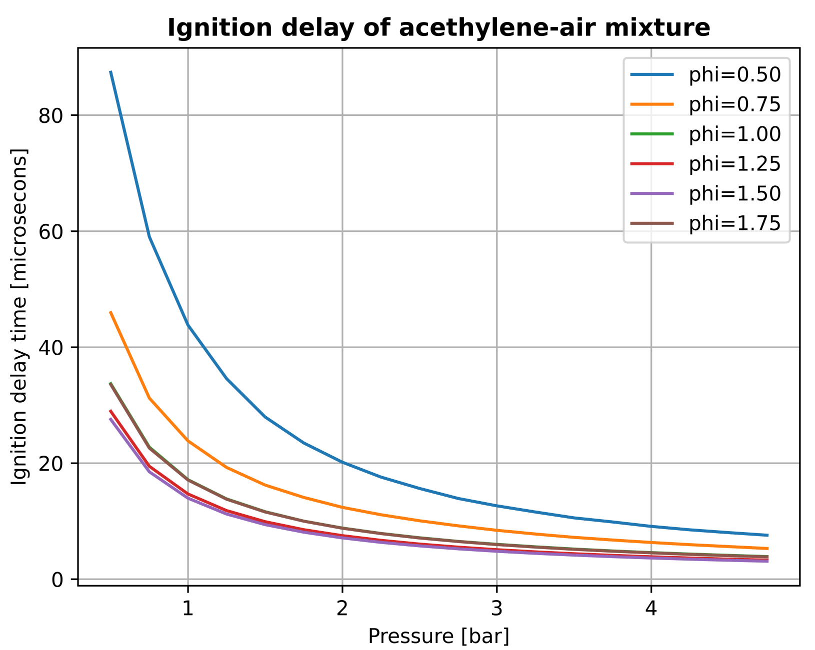


Figure 9: Ignition delay as a function of the pressure for acethylene - air mixture

5 Conclusions

The ignition delay is influenced by the initial temperature, pressure, and equivalence ratio. The plotted data reveals that, in most cases, the ignition delay substantially decreases with increasing temperature or pressure. However, an exception is observed in the case of the ethane-air mixture and acethylene - air mixture under constant pressure with varying temperature. The curves exhibit a characteristic shape, with the ignition delay peaking between 2500 and 3200 K.

Furthermore, it is evident that for a wide range of initial conditions, the ignition delay is shortest around stoichiometry, specifically for slightly fuel-rich mixtures. Poor or extremely rich compositions exhibit difficulties in igniting. It is apparent that higher temperatures and pressures, along with stoichiometric conditions, provide more favorable circumstances for rapid ignition.

6 Bibliography

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[7] https://github.com/WeronikaDziaduch/MKWS?search=1