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## METODY KOMPUTEROWE W SPALANIU

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### **Autoignition of methane - air mixture for different initial temperature, pressure and equivalence ratio**

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## 1 Abstract.

The purpose of the project was to conduct a study of autoignition of a methane air mixture for different initial temperature, pressure and equivalent ratio, using Cantera software. The results of the study are several plots, showing influence of these parameters on autoignition timing and final temperature and a .csv file with all the data.

## 2 Mathematic model.

There are several definitions of autoignition that can be found in the literature. For the needs of the study, we used the one that relies on the temperature gradient: the time of the sharpest temperature increase is spotted as being the autoignition point. In order to catch this point, the step of the simulation was set possibly small –  $10^{-6}s$ . The calculations were held for 10 different temperatures, pressures and  $\phi$  (10x10x10). It took couple of minutes (2-3) to calculate it. The more accurate we want the calculations to be, the more iterations we have to make and the more time it takes. For the purpose of this project, 10x10x10 is more than enough.

## 3 Results and plots.

### 3.1 Results for $P = 1013,25hPa$ , $\phi = 1$ and different initial temperatures.

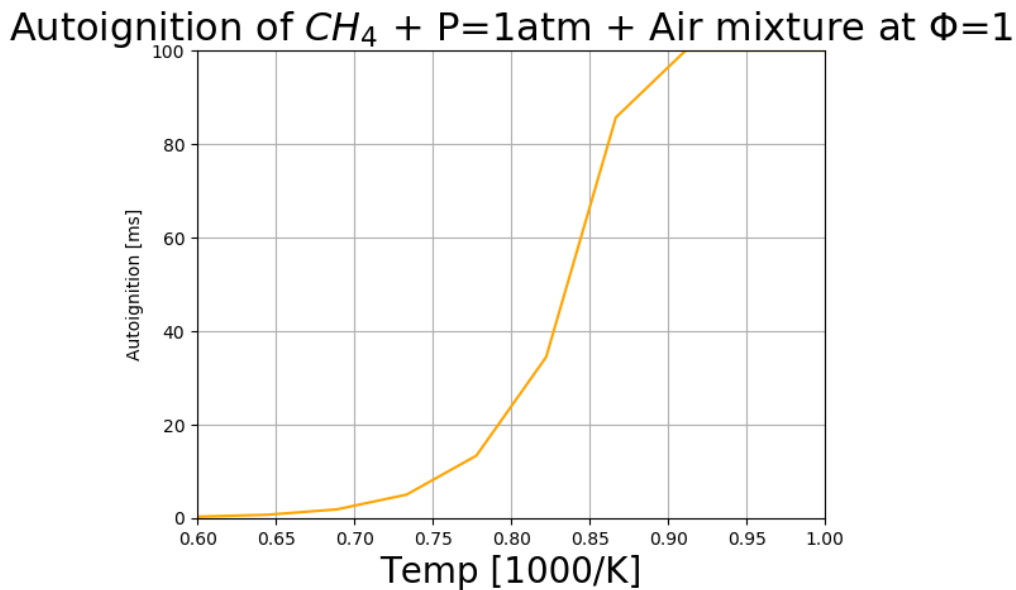


Figure 1: Influence of initial temperature on autoignition timing.

We observe a severe drop of the timing with a rise of the temperature. Autoignition doesn't take place below 1100K.

### Autoignition of $CH_4 + P=1\text{atm} + \text{Air}$ mixture at $\Phi=1$

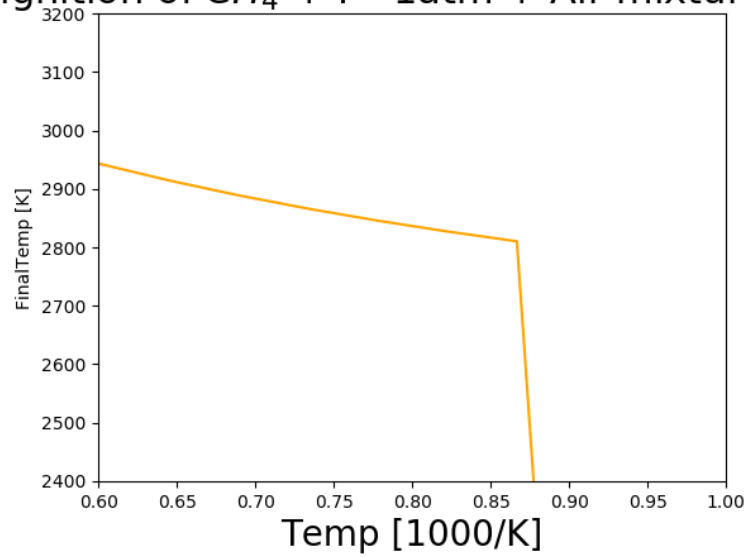


Figure 2: Influence of initial temperature on final temperature.

influence of initial temperature on final temperature. Starting with 1200K, a linear growth of a final temperature is noticed. Below 1200K the growth is unnoticeable or the autoignition doesn't occur.

### 3.2 Results for $T = 1300K$ , $\phi = 1$ and different initial pressure.

### Autoignition of $CH_4 + T=1300K + \text{Air}$ mixture at $\Phi=1$

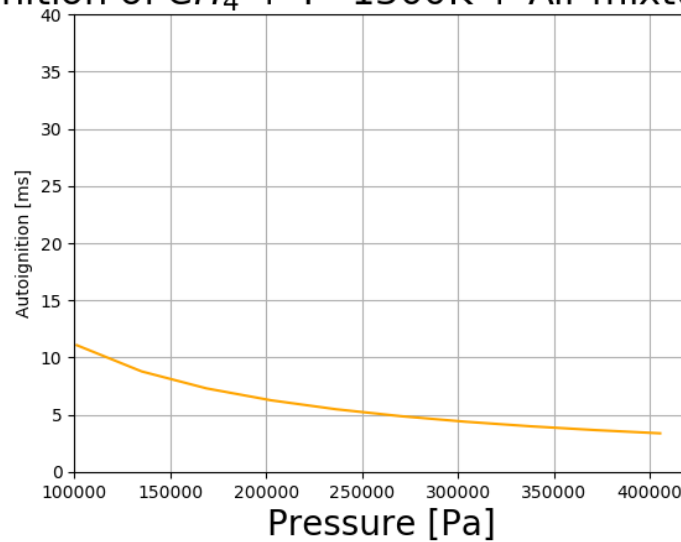


Figure 3: Influence of pressure on autoignition timing.

The time of autoignition decreases for greater pressure values.

### Autoignition of $CH_4$ + T=1300K + Air mixture at $\Phi=1$

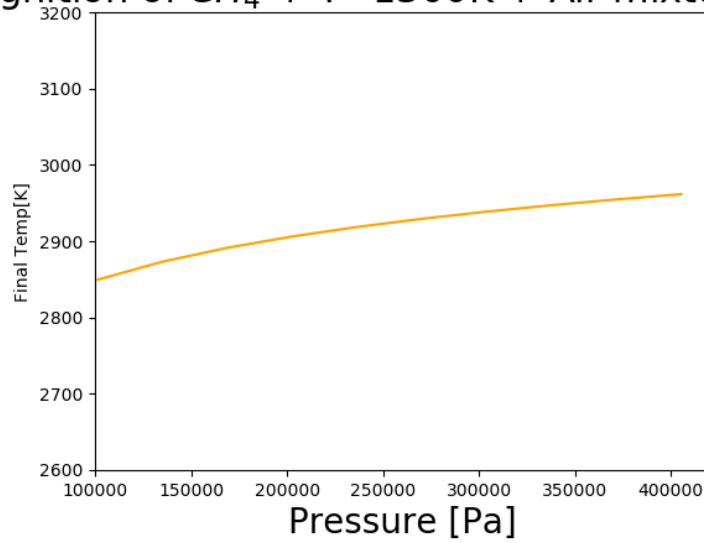


Figure 4: Influence of pressure on final temperature.

The plot shows us, that the final temperature increases with the growth of pressure values.

### 3.3 Results for $T = 1300K$ , $P = 1013,25hPa$ and different equivalent ratio values ( $\phi$ ).

#### Autoignition of $CH_4$ + P=1atm + T=1300K

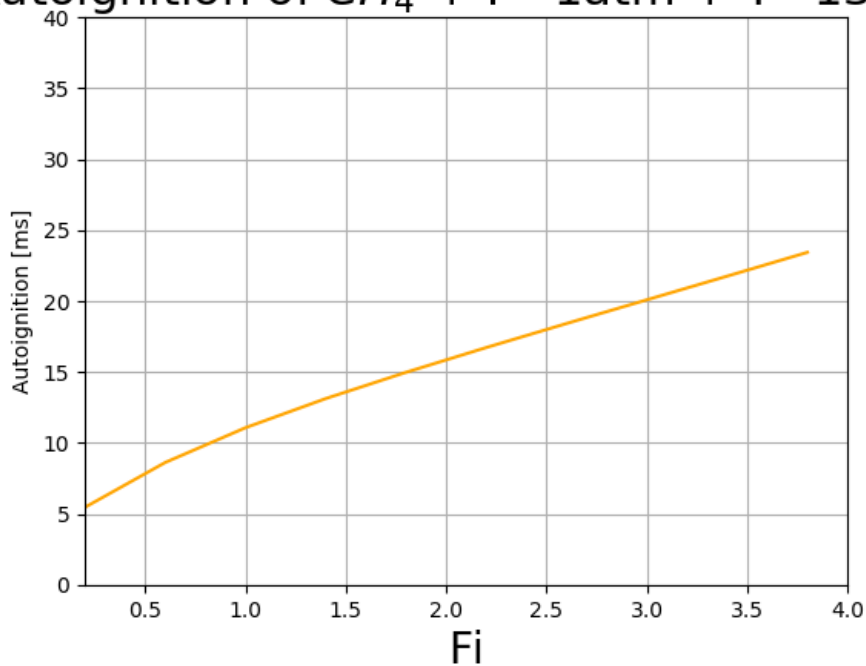


Figure 5: Influence of  $\phi$  on autoignition timing.

We can notice a growth in autoignition timing for greater  $\phi$  values.

## Autoignition of $CH_4$ + P=1atm + T=1300K

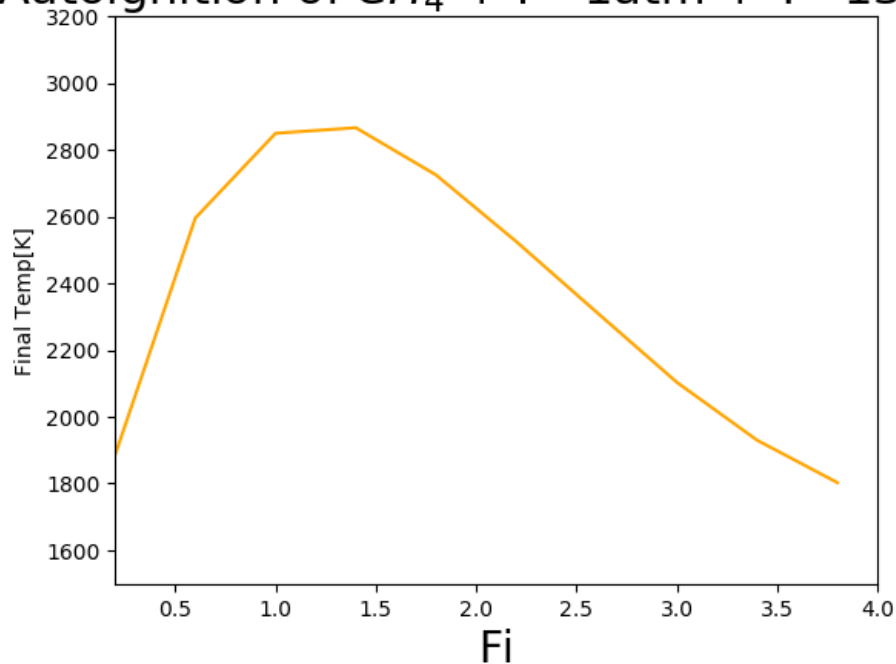


Figure 6: Influence of  $\phi$  on final temperature.

The greatest value of final temperature can be spotted in area of  $\phi = 1$  (2900K). Therefore, it is the optimal value of the coefficient.

## 4 Overall.

The study gives information about the behavior of autoignition as a function of temperature, pressure and  $\phi$ . The definition of autoignition proposed in the mathematical model is the most commonly used one. The data read from the plots are just approximations of the actual state. The more precise data can be read from the .csv file (*MW – Autoignition<sub>Methane</sub>.csv* attached to a report). This file contains information about the lowest temperature of autoignition.

## 5 References.

1. *CANTERA\_HandsOn.pdf*
2. *Wykład\_4\_Cantera.pdf*
3. Prediction of auto-ignition temperatures and delays for gas turbine applications.  
<http://proceedings.asmedigitalcollection.asme.org/proceeding.aspx?articleid=2428119>