Autoignition of the hydrogen and oxygen-nitrogen combinations mixture at 650K

Ewelina Zaremba LiK Metody komputerowe w spalaniu
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Scope

The scope of this examination was to observe the changes of parameters describing autoignition, related to the φ ratio value, and finding a relation between detonation cell width and induction time. This parameters are:
• Induction time [s]
• Chapman - Jouget speed [m/s]
• Exothermic time [s]
• Pressure post shock [Pa]
• Temperature post shock [K]
• Final temperature [K]
• Effective activation energy

Assumptions

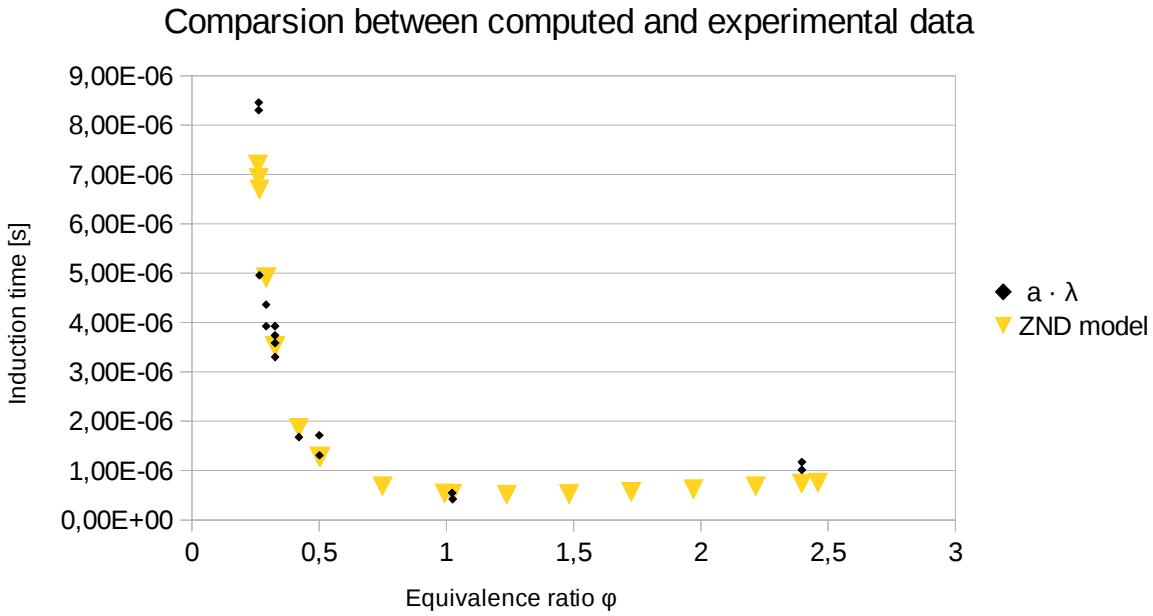
The constant molar sum approach was conducted (it could also be the constant mass sum approach). Calculations were zero-dimensional.

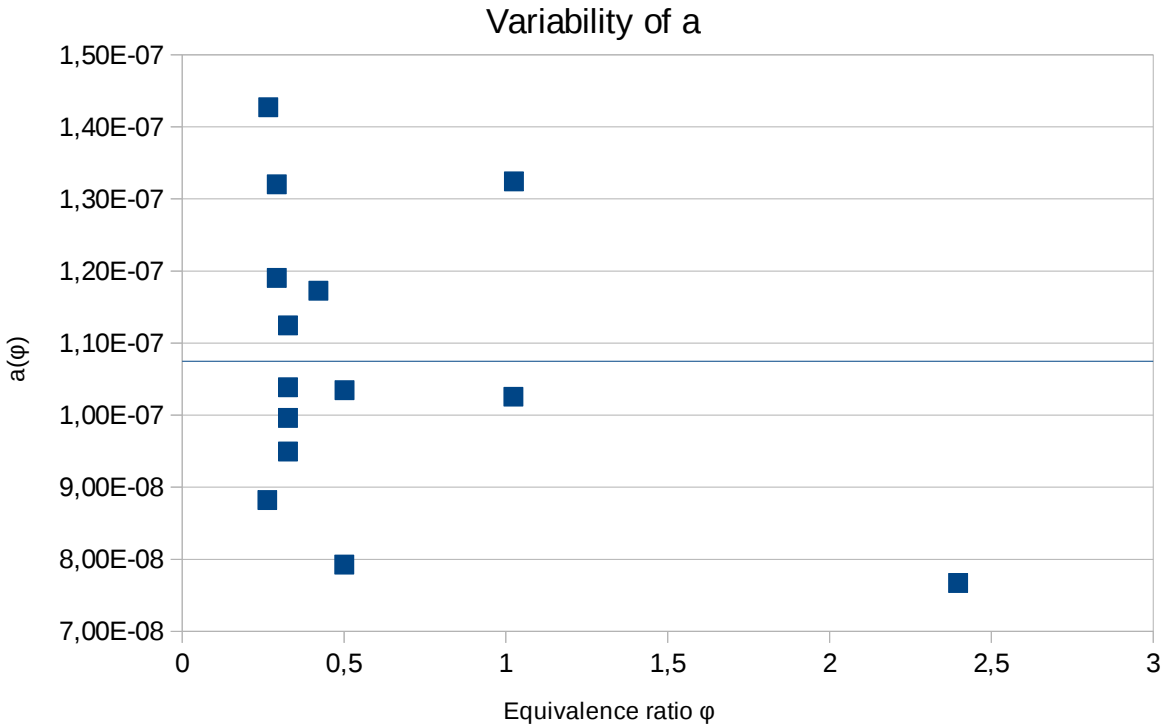
Mathematical model

Build-in Cantera functions and SDToolbox Matlab scripts were used. ZND model was used.
As one of point of this work was to find relation between cell width and induction time, some computation was made. Hypothesis is $t_{ind}(\varphi) = a \cdot \lambda(\varphi)$. Using simple math: $a(\varphi) = t_{ind}(\varphi) / \lambda(\varphi)$.
a is function of φ, because of many possible errors, like determining cell size precision.
For this linear equation an estimator of constant **a** was a mean.

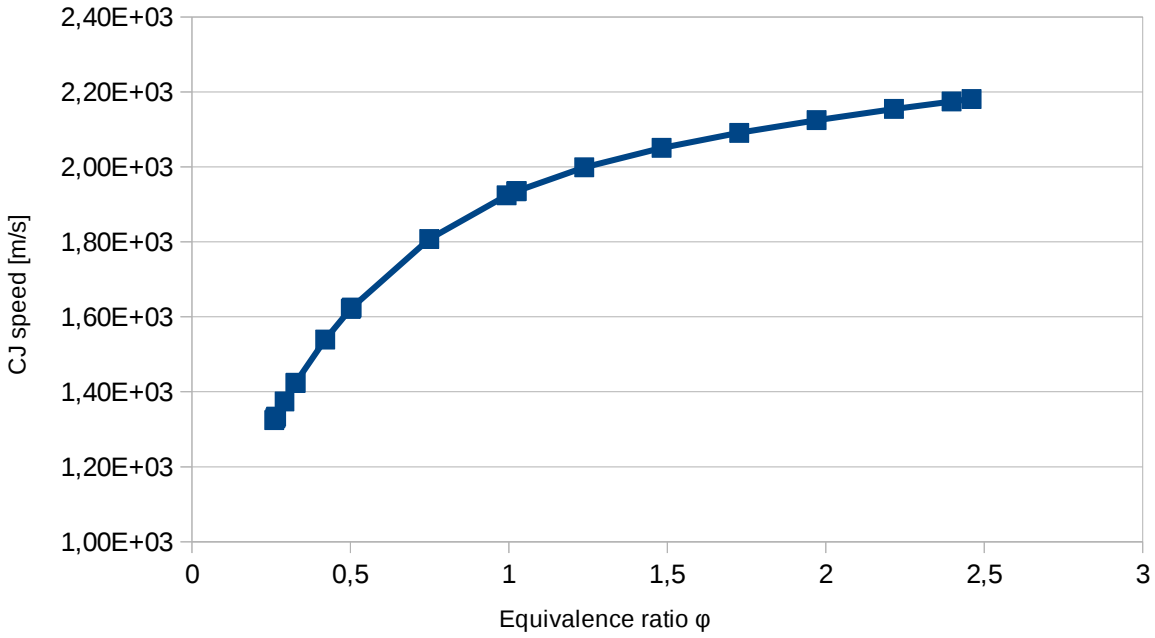
Results

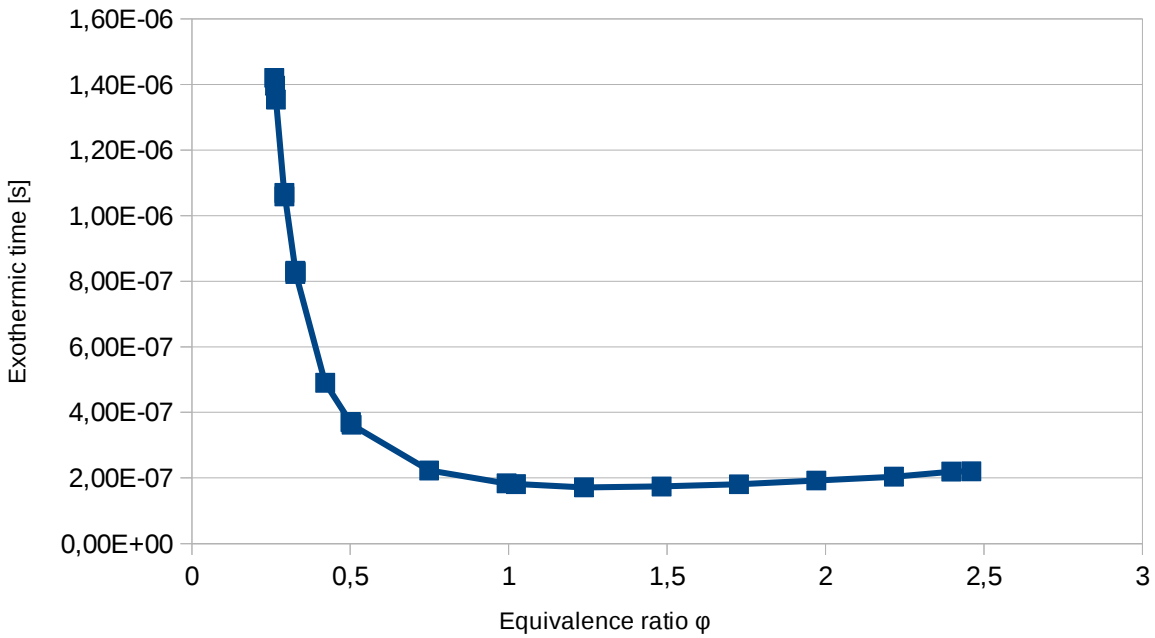
As it is shown on the plots below, the results were obtained in line with expectations.

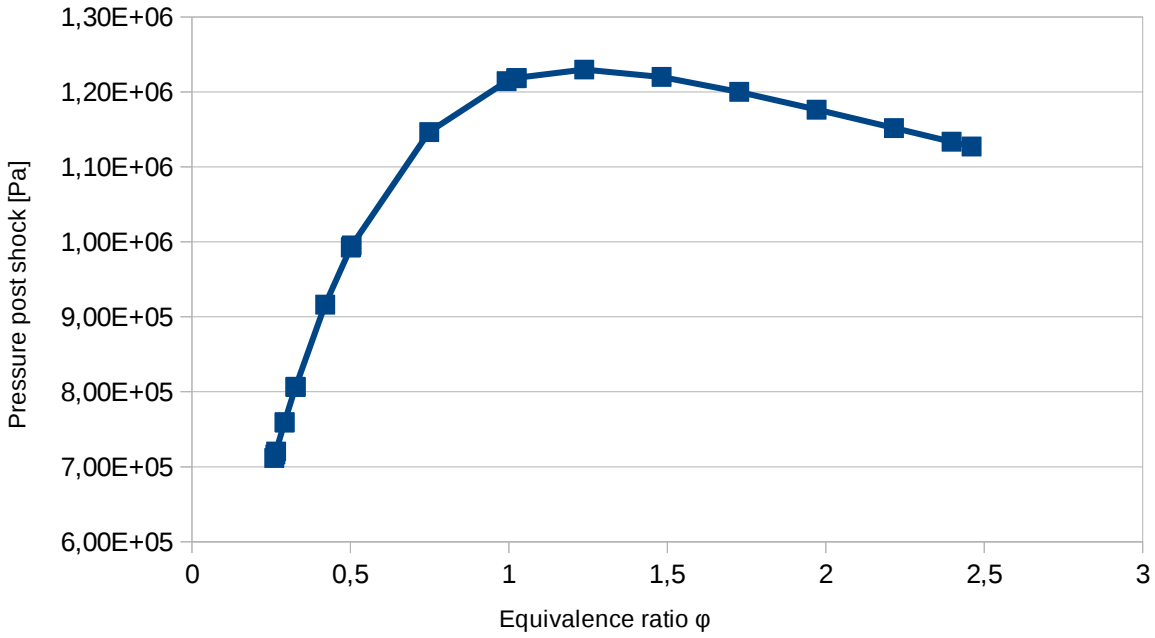


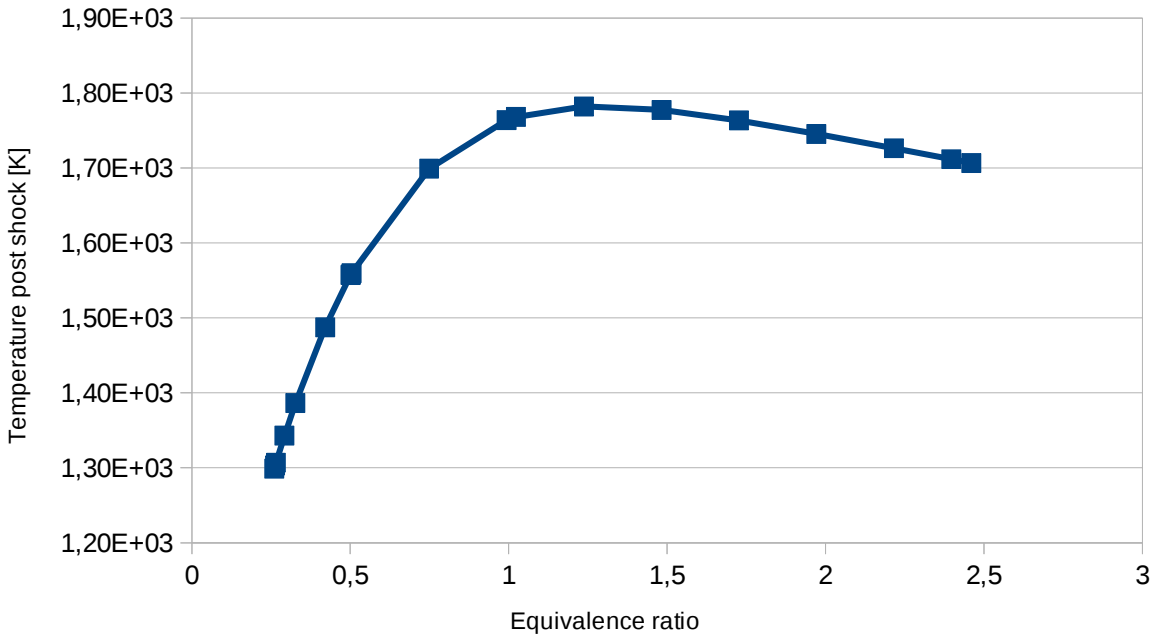


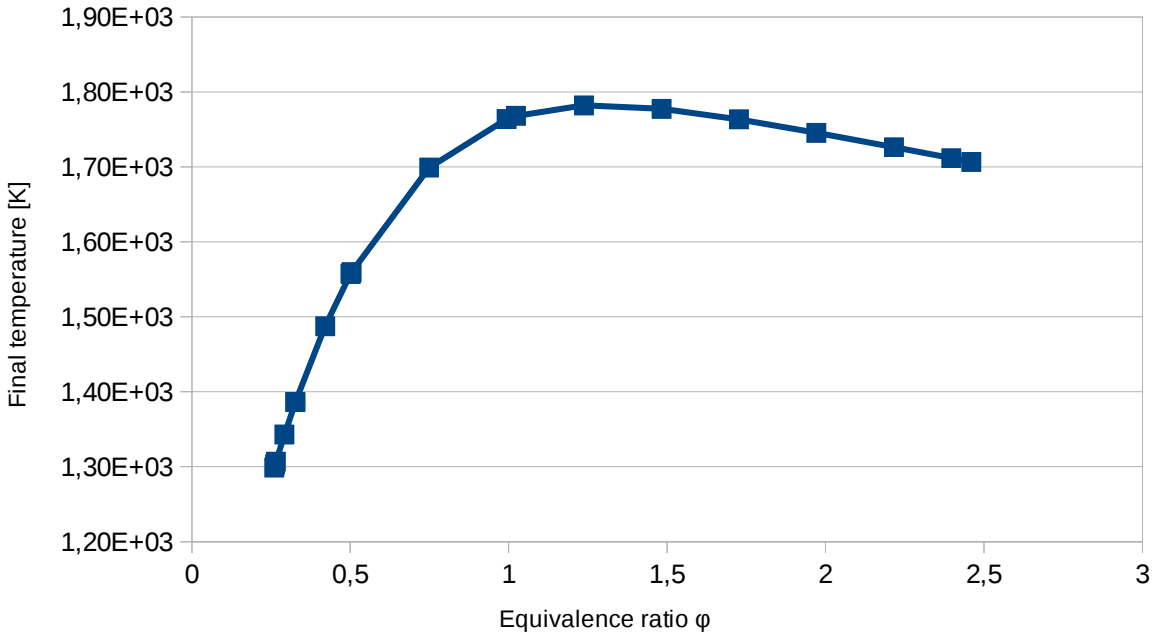
Mean **a** value is 1,074e-7[s/m].
Coefficient of variation is 0,18.

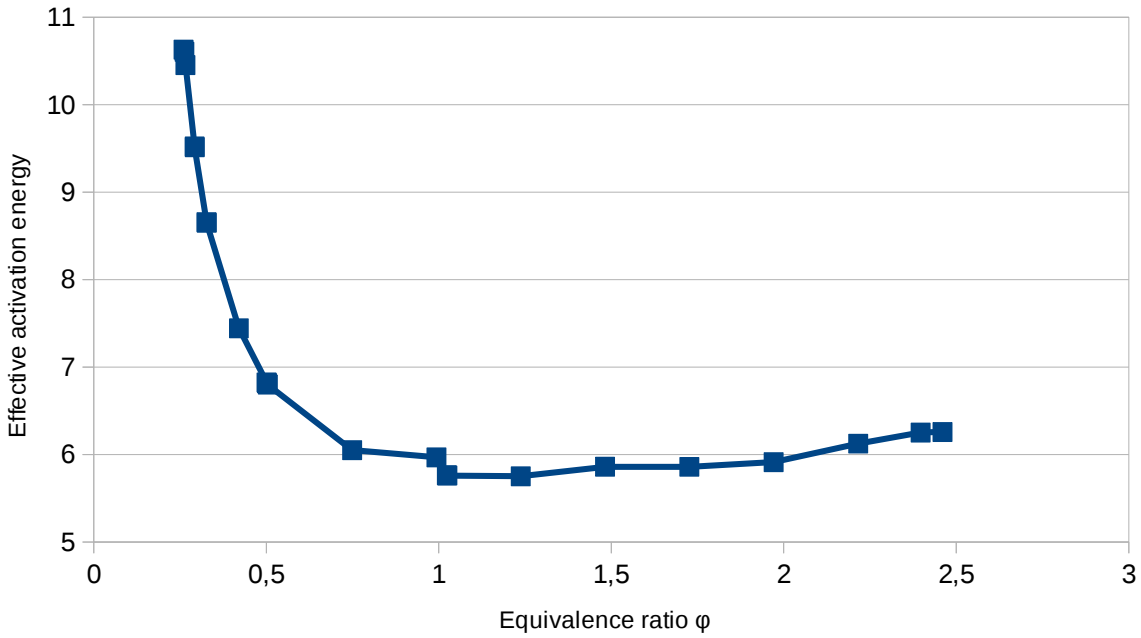

2,40E+03
2,20E+03
2,00E+03
1,80E+03
1,60E+03
1,40E+03
1,20E+03
1,00E+03
CJ speed [m/s]
0
0,5
1
1,5
2
2,5
3
Equivalence ratio φ


1,60E-06
1,40E-06
1,20E-06
1,00E-06
8,00E-07
6,00E-07
4,00E-07
2,00E-07
0,00E+00
Exothermic time [s]
0
0,5
1
1,5
2
2,5
3
Equivalence ratio φ


1,30E+06
1,20E+06
1,10E+06
1,00E+06
9,00E+05
8,00E+05
7,00E+05
6,00E+05
Pressure post shock [Pa]
0
0,5
1
1,5
2
2,5
3
Equivalence ratio φ


1,90E+03
1,80E+03
1,70E+03
1,60E+03
1,50E+03
1,40E+03
1,30E+03
1,20E+03
Temperature post shock [K]
0
0,5
1
1,5
2
2,5
3
Equivalence ratio





Summary

Our x axis on every plot represents phi ratio.
Experimental data matches well for computation model.
Extremes for most computed plots are for φ = 1.
Characteristics of final temperature and maximum pressure results from the different proportions of ingredients.
Effective activation energy drops fast for φ in (0.25, 0.5) as like exothermic time.

References

[1] CANTERA Tutorials - A series of tutorials to get started witlyxh the python interface of Cantera version 2.1.1, Anne Felden
[2] Division of Engineering and Applied Science California Institute of Technology, Cantera Workshop, July 25, 2004, D. G. Goodwin
[3] Spalanie, 1969, Stanisław Wójcicki
[4] Experimental data obtained from: http://shepherd.caltech.edu/detn_db/html/db_121.html