

Ignition delay computation of methane in oxygen

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Abstract

Here is the raport of the computation of ignition delay of methane in oxygen

1 Introduction

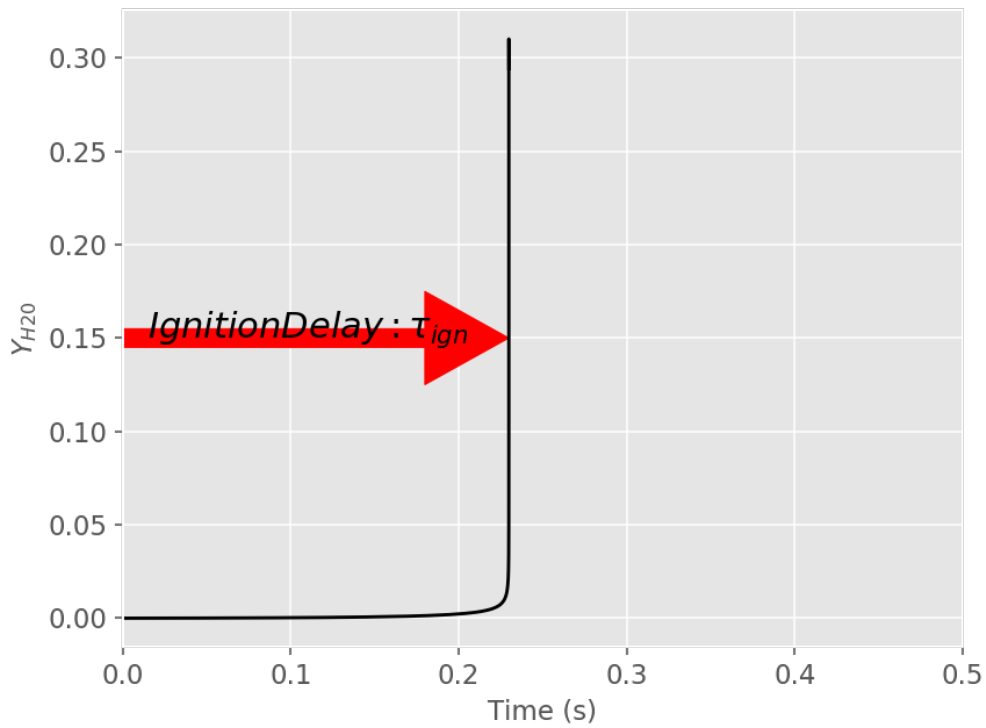
Ignition delay time or reaction time is one of the most important parameters characterizing the combustion process of different fuels and thus is very important for combustion modeling. Accurate calculation of the ignition delay time, especially for the combustion process with a variety of fuel blends in gas turbines and other combustion engines, is a complicated procedure because of the complex interaction between flows and chemical kinetics. In these case we will compute ignition delay time of methane in oxygen for various temperatures.

2 Model description

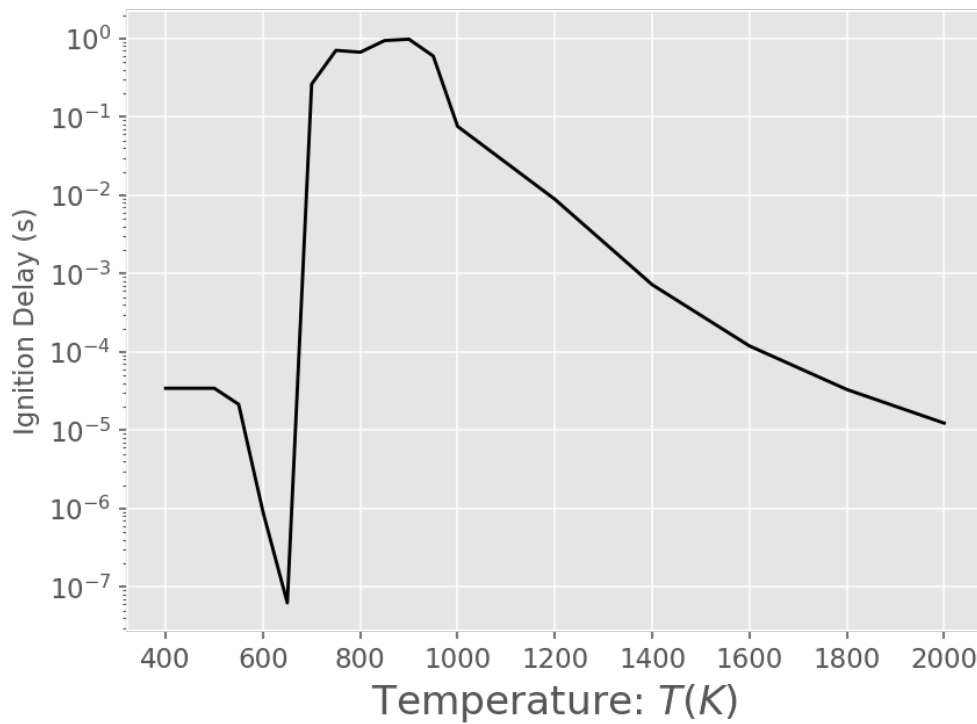
GRI-Mech 3.0 is a widely-used reaction mechanism for natural gas combustion. It contains 53 species composed of the elements H, C, O, N, and/or Ar, and 325 reactions, most of which are reversible. GRI-Mech 3.0, like most combustion mechanisms, is designed for use at pressures where the ideal gas law holds.

3 Results analysis

Initial parameters: $T=1000\text{K}$ $p=1013,25\text{Pa}$ For these parameters computed ignition delay time is 0,2298 seconds.



On this plot we can see that in 0,2298 seconds there is rapid increase in quantity of water particles. That's because from reaction of methane with oxygen, it is inevitable that we will receive water, so that we decided to analyze presence of water in reactor.



On this plot we can see that it isn't true that with the increase of temperature shortens ignition delay times. Between 600-900K we've got rapid increase. Shortest ignition delay time is for 650K, and it's $6,25 \times 10^{-8}$ s.

4 Conclusion

Ignition delay time varies in a wide range, it depends on initial temperatures. Also it is important that computation reproduce empirically observed Negative Temperature Coefficient behavior. Analysis of chemical composition of reactors is a good way to detect if ignition took place in the engine.

5 References

- <https://link.springer.com/content/pdf/10.1007/s11434-010-4345-3.pdf>
- [https://github.com/Cantera/cantera-jupyter/blob/master/reactors/batch reactor ignition delay NTC.ipynb](https://github.com/Cantera/cantera-jupyter/blob/master/reactors/batch%20reactor%20ignition%20delay%20NTC.ipynb)