Politechnika Warszawska

Wydział Mechaniczny Energetyki i Lotnictwa

Metody Komputerowe w Procesach Spalania

Hydrogen and Methane ignition delay comparison

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1 Introduction

Subject of this project was checking the ignition delay of hydrogen and methane in the air, depending on starting temperature and pressure for stoichiometric mixtures. If we want to use hydrogen or methane as a fuel, ignition is the most important factor to optimize burning process. Using my code the temperature rise and ignition delay can be computed for different initial parameters.

2 Model description

2.1 Software

Cantera is an open-source suite of object-oriented software tools for problems involving chemical kinetics, thermodynamics, and/or transport processes. The software automates the chemical kinetic, thermodynamic, and transport calculations so that the users can efficiently incorporate detailed chemical thermo-kinetics and transport models into their calculations.

The code utilizes object-oriented concepts for robust yet flexible phase models, and algorithms are generalized so that users can explore different phase models with minimal changes to their overall code. Currently, Cantera can be used from Python and Matlab, or in applications written in C/C++ and Fortran 90. Cantera also provides a limited number of solvers for time-dependent reactor networks and steady one-dimensional reacting flows.

In this case Python have been used.

2.2 Gas model

A Reactor gas model has been used. A Cantera Reactor represents the simplest form of a chemically reacting system. It corresponds to an extensive thermodynamic control volume V, in which all state variables are homogeneously distributed. The system is generally unsteady, i.e. all states are functions of time. In particular, transient state changes due to chemical reactions are possible. However, thermodynamic (but not chemical) equilibrium is assumed to be present throughout the reactor at all instants of time. Volume wasn't fixed. Initial state was specified by pressure and temperature, mixture was stoichiometric.

2.3 Actions

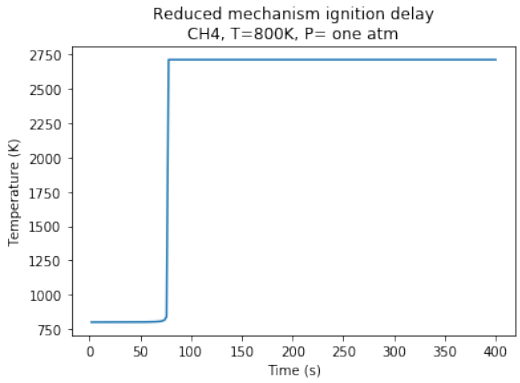
Temperature and pressure can be changed in the code, then the time step can be adjusted to fit between start and start of the ignition.

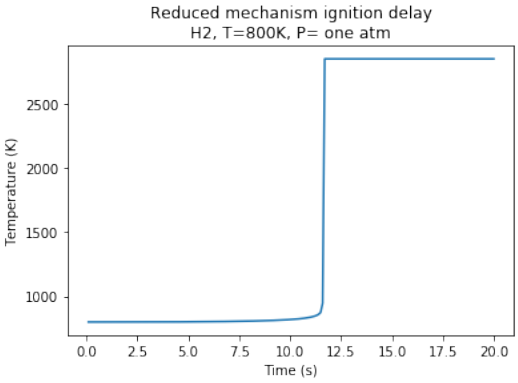
3 Results

Ignition delay times were computed for three starting temperatures and for three pressures respectively: 800K, 1000K, 1200K and one atm, two atm and three atm for both gases.

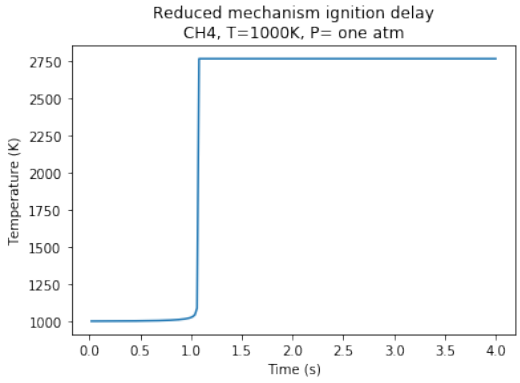
3.1 One atm

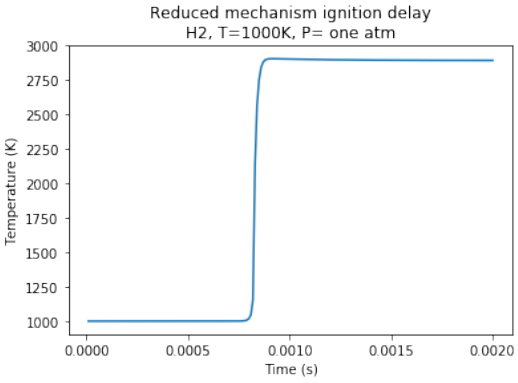
3.1.1 800K



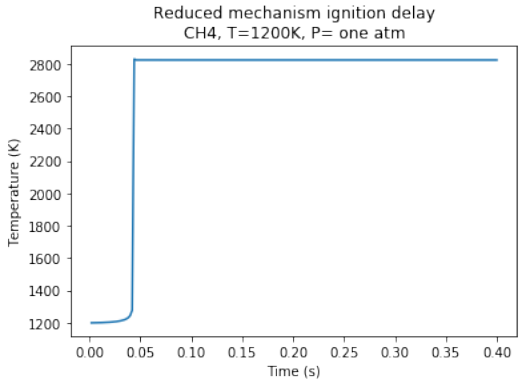


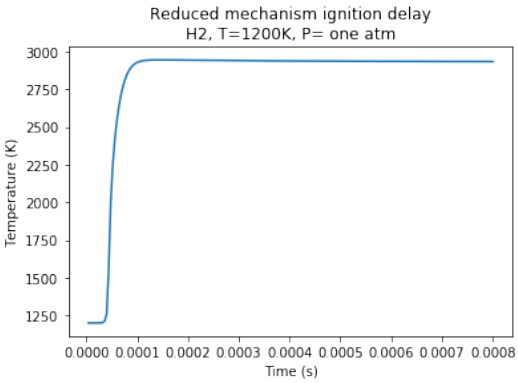
3.1.2 1000K





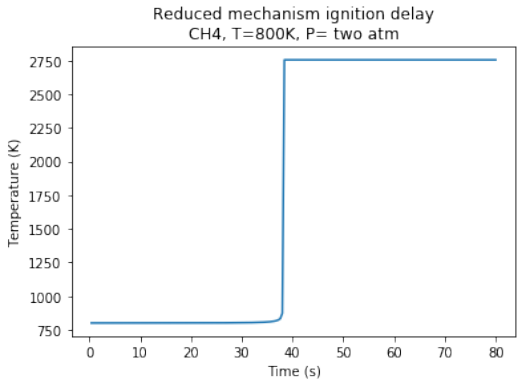
3.1.3 1200K

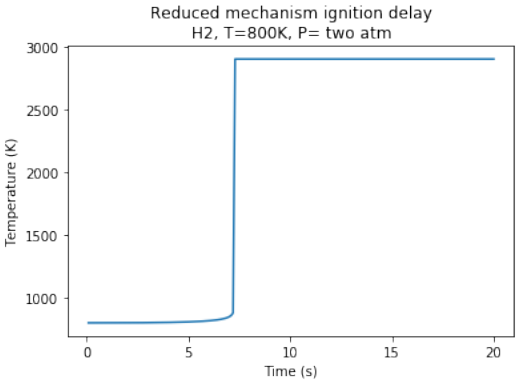




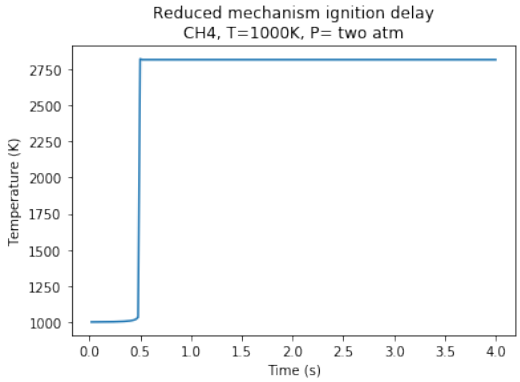
3.2 Two atm

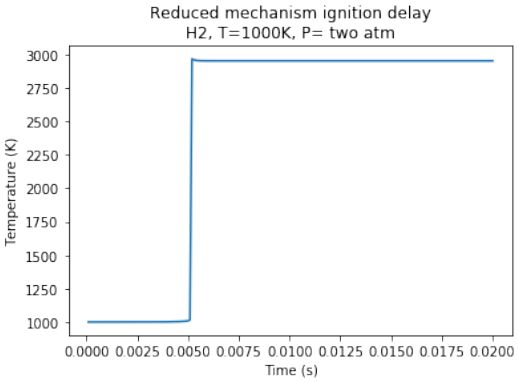
3.2.1 800K



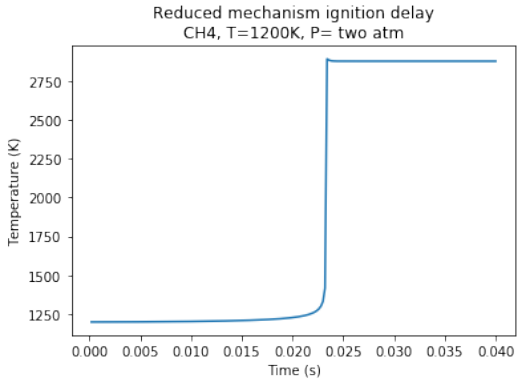


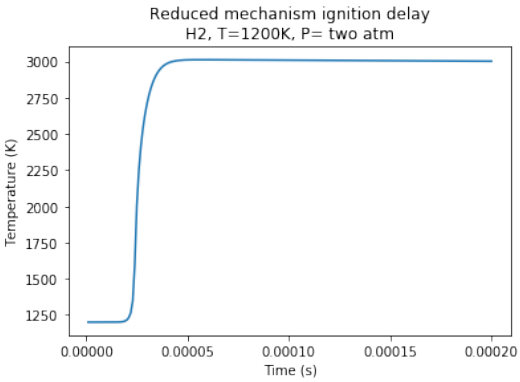
3.2.2 1000K





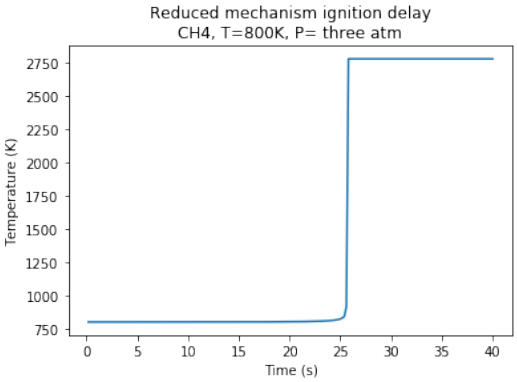
3.2.3 1200K

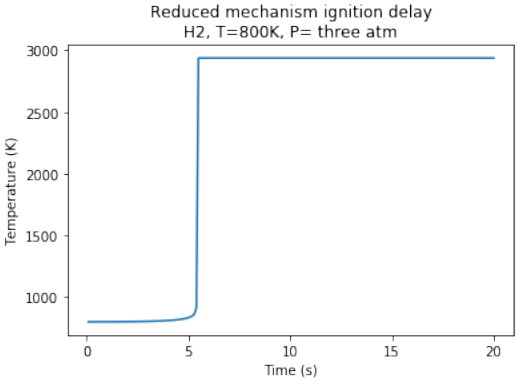




3.3 Three atm

3.3.1 800K





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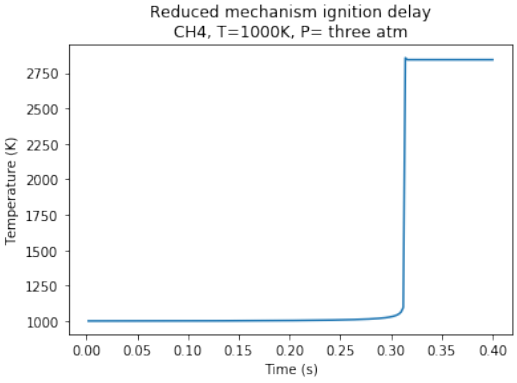
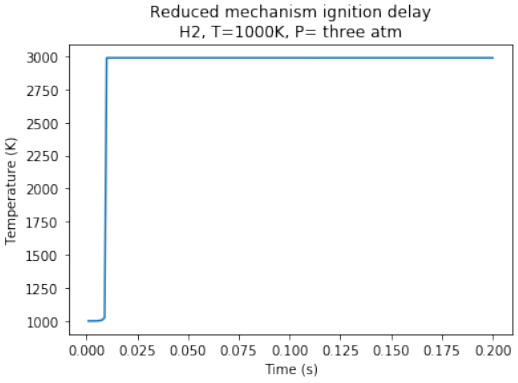
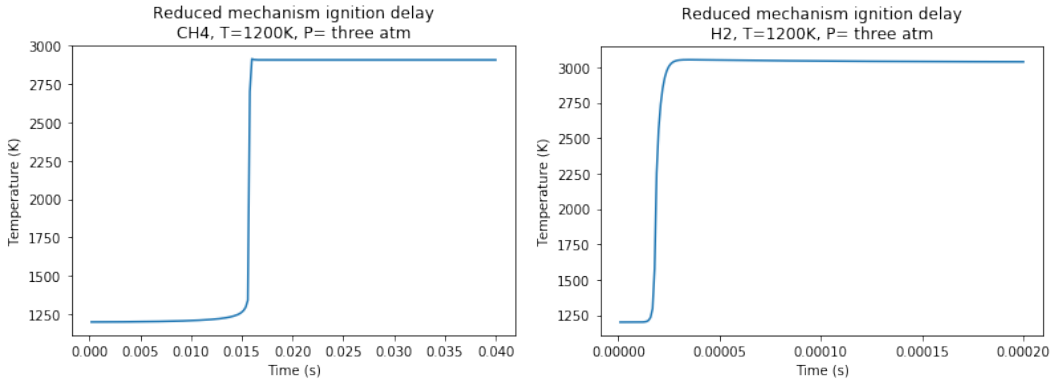




3.3.3 1200K



4 Conclusion

As can be seen the ignition delay time depends as well well on temperature as on pressure. The higher temperature the faster the reaction is. The Same thing can be said about pressure. What is also noticeable is fact that hydrogen reacts much faster and has significantly shorter ignition dealay times in all considered conditions.

5 Bibliography

- MKWS lectures
- Cantera website
- Overleaf website