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Combustion of mixtures with different concentrations of nitromethane and air

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Chapter 1

1.1 Introduction

The purpose of this report is to analyze the differences in the combustion of different nitromethane-air mixtures. The analysis has been conducted to obtain results of pressure, temperature and gases composition.

1.2 Method description

The analysis has been implemented in Python using Cantera library with reaction mechanism Fuller-2021[2] which is a detailed mechanism for compounds containing nitrogen.

Created model simulates a tank with a volume of 0.0005 m^3, the initial temperature of the fuel-air mixture is 700 K at a pressure of 1 atm. The mixture is ignited by a simulated spark. Unfortunately there is no realistic way to model ignition in a zero-D system, where the concept of a 'spark' simply can't exist. In order to create similar result a stream of free hydrogen radicals is being injected.

Hydrogen is injected using Gaussian pulse. A Gaussian pulse (shown in *figure 1.1*) is shaped as a Gaussian function and is produced by the impulse response of a Gaussian filter.

Equation (1.1) describes pulse used in the simulation. Each mixture is ignited by a spark simulated in the same way. Using $1.0e-8$ kg of hydrogen at 1000 K.

$$f(x) = a \exp\left(\frac{-(t-t0)^2}{(2\ \text{fwhm}^2)}\right) \tag{1.1}$$

Where:

- **fwhm** is full width at half maximum and equals 0.1[s]
- **t0** is peak point, equals 1.0 [s]

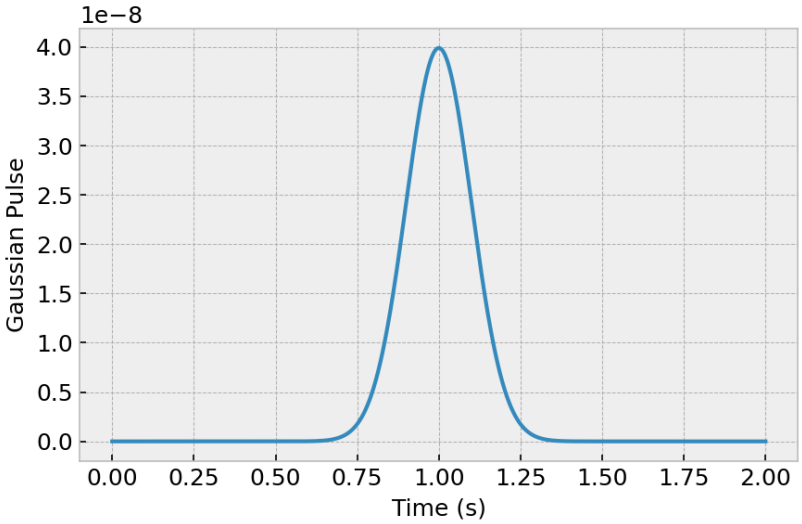

Figure 1.1: Gaussian pulse used to supply hydrogen.

- **a** is the amplitude describing the mass of the substance that is delivered [kg]

1.3 Combustion of a stoichiometric mixture

Let's analyze combustion of a stoichiometric mixture of nitromethane and air. Equation for nitromethane and oxygen combustion is as follows:

$$4\,CH_3NO_2 + 5\,O_2 \longrightarrow 4\,CO_2 + 6\,H_2O + 4\,NO \tag{1.2}$$

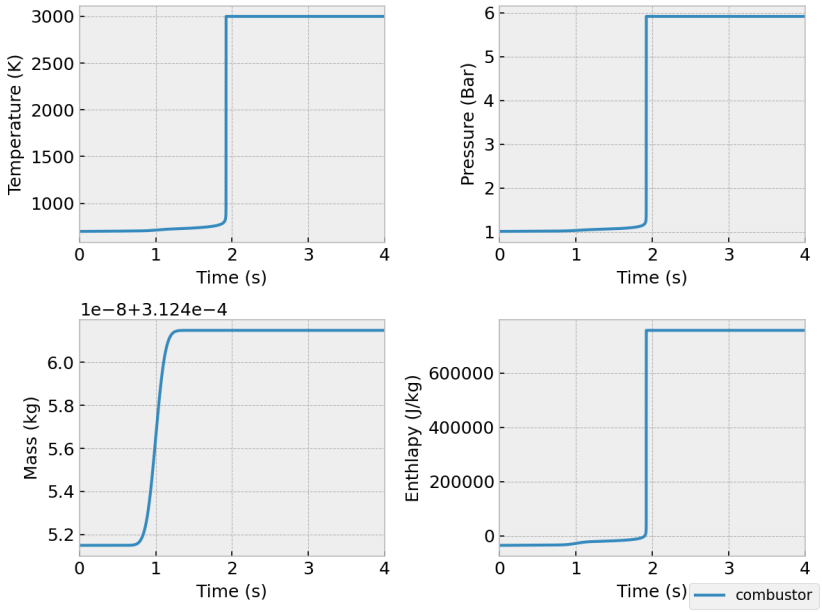

Figure 1.2: Parameters over time for stoichiometric mixture.

The simulation starts with with filling the reactor with air-fuel mixture acording to the ϕ ratio. Approximately at $t = 1.30$ injection of free hygrogen radicals is finished. As you can see from this point, the temperature in the reactor slowly starts to rise, so that at $t = 1.9$ it explodes. The reactor reaches a steady state around $t = 1.93$. *Figure 1.2* shows the course of the combustion process of the stoichiometric mixture.

Figure 1.3 shows gas composition during simulation. As can be seen combustion happens almost instantly. When nitromethane is burned, various nitrogen oxides and a significant amount of carbon dioxide are produced. Since the simulation can use 837 different molecules [2], we do not limit the modeled reaction to nitromethanol combustion reaction products only. We can observe in the reactor such compounds as the mentioned nitrogen oxides or carbon monoxide.

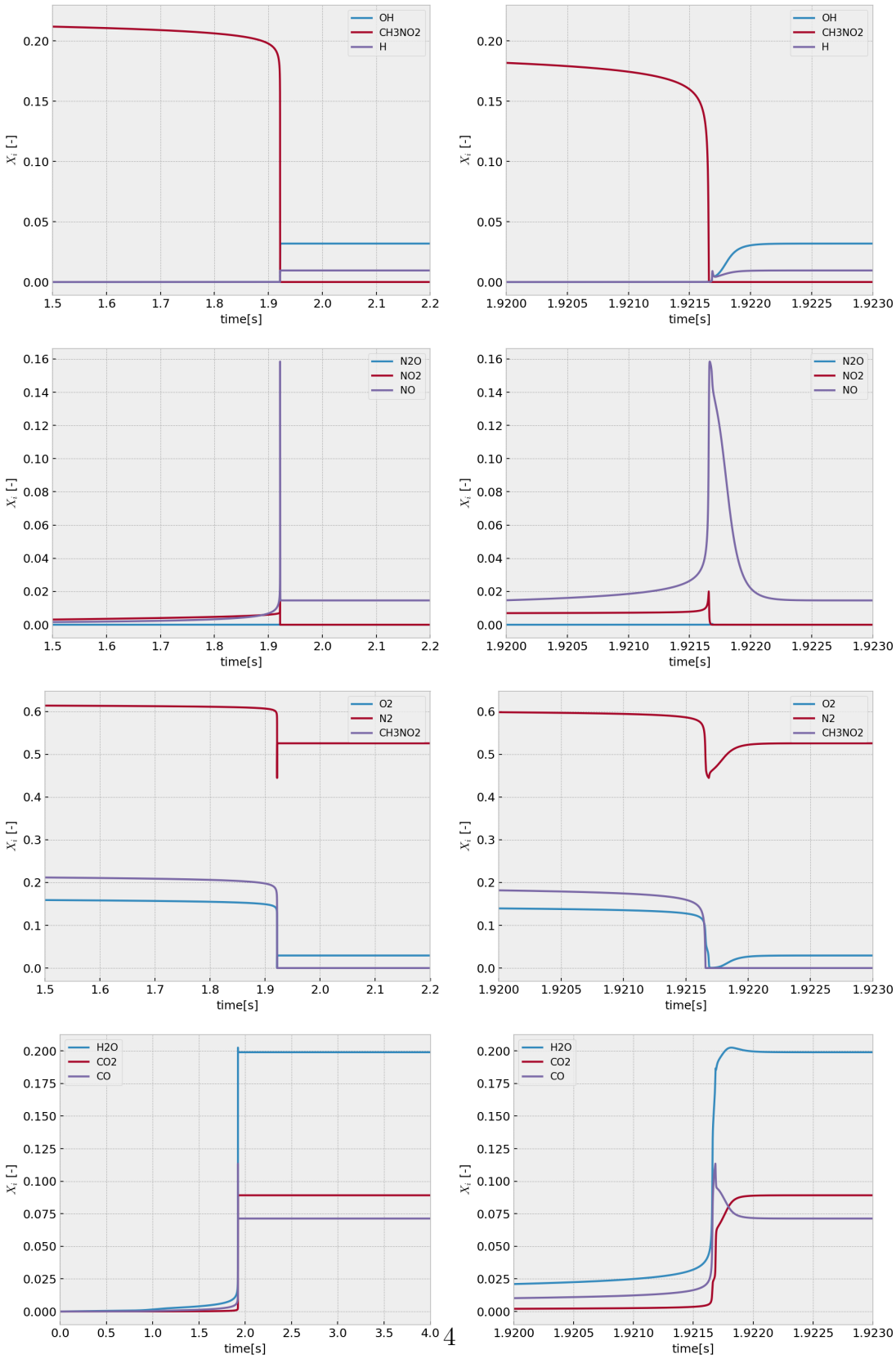

Figure 1.3: Gas composition in the reactor over time. Graphs on the right are stretched on horizontal axis.

1.4 Results

For each value of $\phi \in (0, 1)$ a mixture is created and a simulation is performed. Due to the complexity of the calculations and the time that is needed to perform them, 15 values of ϕ in a chosen range were selected.

ϕ				
0.1	0.1643	0.2286	0.2929	0.3571
0.4214	0.4857	0.55	0.6143	0.6786
0.7429	0.8072	0.8714	0.9357	1.0

The graph below shows the differences in the temperature and pressure depending on the fuel concentration

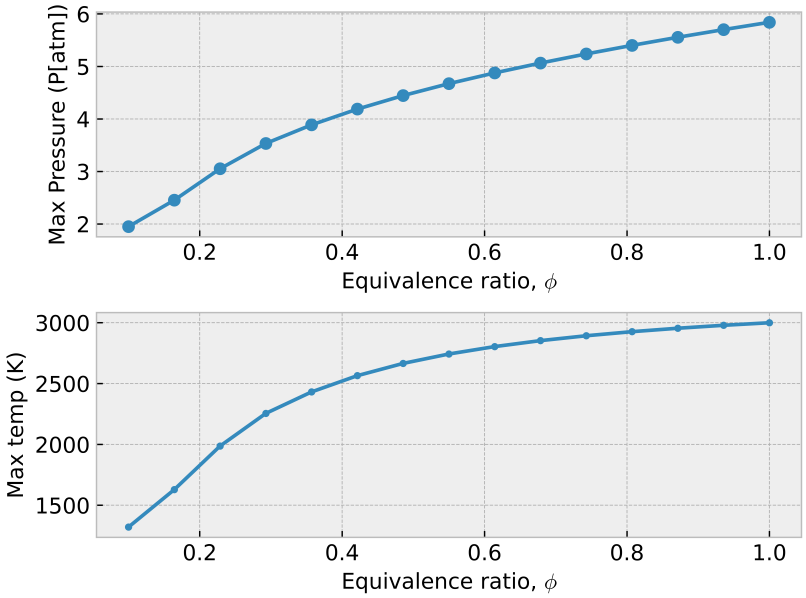

Figure 1.4: Highest temperature and pressure for each mixture created.

As we can see the combustion is proceeding as expected. Maximum pressure and temperature increase as ϕ increases. *Figure 1.3* shows big amounts of nitrogen oxides being involved in the reaction.

It should be noted that we are unable to simulate the combustion of nitromethane for mixtures with a ratio greater than 1. This is due to the fact that the thermal data we use is unable to perform calculations for such a complex reaction at temperatures above 3000 K. However, if we limit the reaction products to only carbon dioxide, water and nitrogen oxide, we can find the flame temperature resulting from these reactions [1].

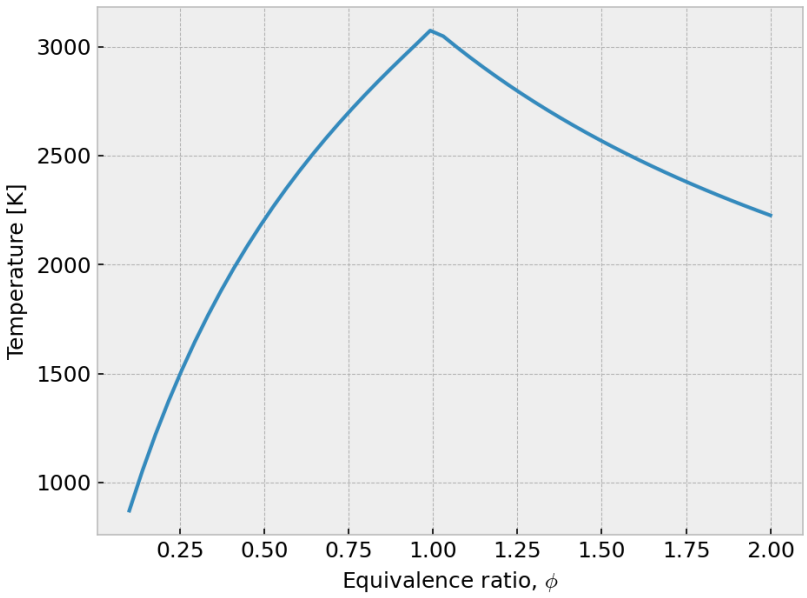

Figure 1.5: Flame temperature for complete combustion.

Figure 1.5 shows that both simulations achieve similar results. The simulation with limited list of products reaches a slightly higher temperature. This may be due to additional chemical reactions that take place in the gas formed by the Fuller mechanism.

Bibliography

[1] Flame temperature, 2023.

[2] Mark E. Fuller, Philipp Morsch, C. Franklin Goldsmith, K. Alexander Heufer. The impact of NOx addition on the ignition behavior of n-pentane. *Reaction Chemistry & Engineering*, 6:2191–2203, 2021.