WARSAW UNIVERSITY OF TECHNOLOGY

THE FACULTY OF POWER AND AERONAUTICAL ENGINEERING

COMPUTATIONAL METHODS IN COMBUSTION

Explosion Parameters of Methane-Air, Ethane-air and Propane- air mixtures

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1 Introduction

Aim of this project is to show explosion parameters of methane-air, ethane-air and propane-air mixtures. In order to calculate these parameters a python library cantera was used.

The calculations have been conducted for a constant volume zero dimensional chamber containing a fuel air mixture with the equivalence ratio ranging from 0.1 to 10.

2 Literature review

2.1 Gieras, Marian. "Proces wybuchu." Spalanie, 2021, Warsaw University of Technology. Lecture.

This lecture has covered various types of explosions, including chemical explosions that are the topic of this report. According to this lecture following explosion parameters should be calculated:

- Maximum explosion pressure
- Maximum explosion pressure rise rate
- Optimal explosion concentration
- Lower explosion boundary
- Higher explosion boundary

3 Method description

The experiment will be conducted in cantera's Ideal Gas Reactor. This is a constant volume reactor that allows for calculations of other thermodynamic variables.

3.1 mixture preparation

The reactors chamber is filled with fuel air mixture with predetermined thermodynamic variables. The number of moles of each compound is calculated based on the combustion, ideal gas equation and a set equivalence ratio.

3.2 Ignition

For an ignition a spark is introduced, which is achieved in the code by rising temperature to 1200 K with keeping density constant. This model of ignition is far from being perfect as the heat is introduced to the all the gas at once, while in reality a small amount of energy is introduced locally, and the further mixture ignition is caused by heat introduced by combustion.

3.3 Combustion

Combustion calculations are conducted using cantera library for python. Calculations are conducted in the reactor module. The calculated values in the next step are based on the chemical composition of the mixture and values of thermodynamic variables in a given moment of time.

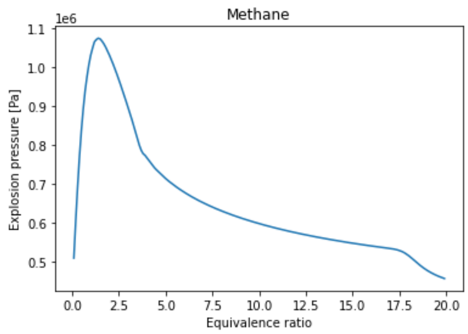
3.4 Data processing

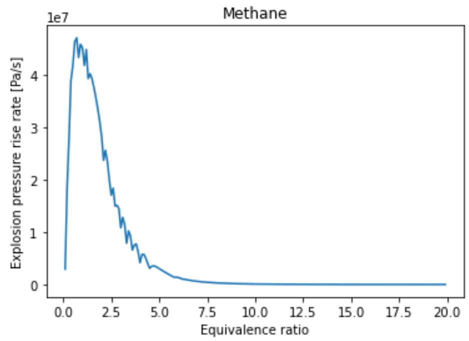
The result of combustion parameters is a 3x(number of steps) matrix. The first row contains consequent time steps, the second row contains the pressure co responding with the time step in the first row, the third row contains the pressure rise rate in the given time step.

The new matrix is introduced that contains the explosion pressure, explosion pressure rise rate and corresponding equivalence ratio. The explosion parameters calculations are based on this matrix.

4 Results

4.1 Methane





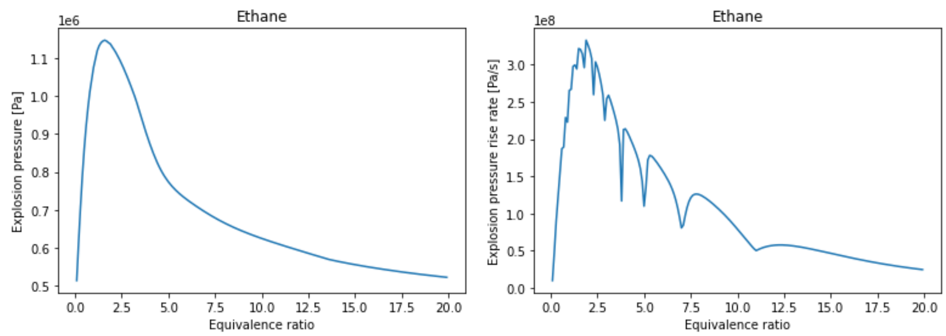
- Maximum explosion pressure = $1.07 MPa$
- Maximum explosion pressure rise rate = $47 MPa/s$
- Optimal explosion concentration = $0.128 Veq = 1.4$
- Lower explosion boundary = 0.01
- Higher explosion boundary = 0.67

According to the PN.EN 15967 norm the maximum explosion pressure of methane is equal to 0.83 MPa, the maximum explosion pressure rise rate is equal to 7.8 MPa/s and the optimal explosion concentration is 0.105 V.

The results of calculations are different than the results of the experiment, however it should be noted that the calculations were conducted for different starting conditions, as the temperature has been artificially risen.

The explosion boundaries for methane are 0.05 and 0.15. The values returned by the program are the maximal and the minimal calculated equivalence ratio.

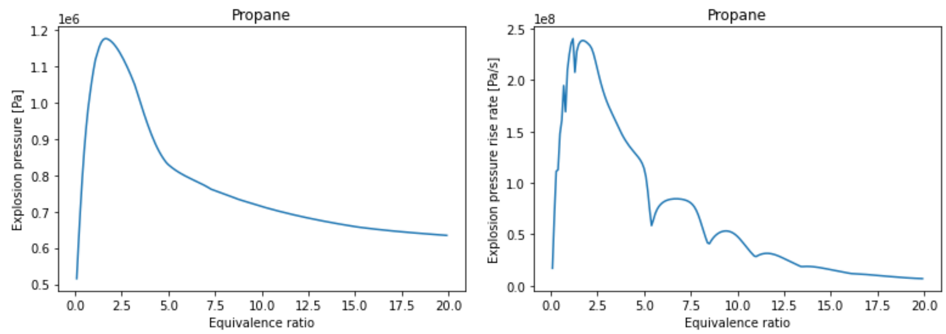
4.2 Ethane



- Maximum explosion pressure = $1.15 MPa$
- Maximum explosion pressure rise rate = $33 MPa/s$
- Optimal explosion concentration = $0.088 Veq = 1.6$
- Lower explosion boundary = 0.01
- Higher explosion boundary = 0.54

Similarly to the previous example the explosion boundaries are the maximal and minimal calculated instances. Compared to methane, the maximum explosion pressure for ethane is higher, while the maximum explosion pressure is lower. It could mean that the more complicated chain of ethane releases more energy, but on a lower rate.

4.3 Propane



- Maximum explosion pressure $= 1.18MPa$
- Maximum explosion pressure rise rate $= 24MPa/s$
- Optimal explosion concentration $= 0.067Veq = 1.7$
- Lower explosion boundary $= 0.004$
- Higher explosion boundary $= 0.46$

The maximum explosion pressure is higher than for methane and ethane, while the maximum explosion pressure rise rate is lower. Again wee see that the optimal explosion concentration is lower than for methane and ethane.

5 Conclusions

5.1 Results analysis

The explosion pressure, and explosion pressure rise rate graphs have similar shapes which means that the maximum explosion pressure occurs for the same mixture as the maximum explosion pressure rise rate. This is an important factor that showcases why chemical explosions are dangerous and certain mixture concentrations should be avoided while storing explosive gases.

The explosion pressure reaches the highest values for the optimal explosion concentration. This concentration is higher than the stoichiometric concentration.

5.2 Method

The chosen method has resulted in the overestimation of parameters. The differences to experimental data stem from a couple of factors. The chosen reactor model conducts reactions in the zero dimensional space. Subsequently the ignition model introduces heat to the entire volume of the chamber and the reaction starts in the whole volume. The result of this is an order of magnitude higher maximum explosion rise rate. The ignition model also introduces much more energy to the system then a local spark would resulting in higher maximum explosion pressure.

As a result of factors listed above it is pointless to study explosion boundaries with this model. The explosion boundaries are caused by either not introducing enough heat to sustain combustion, or too little of the oxidiser being available. In order to study explosion boundaries one should consider creating a multidimensional reactor, however the calculation cost would drastically increase.