Ignition Delay Time

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1 Introduction

Since fossil fuel is depleting and automotive emission regulation is strengthening, researches are paying increasing attention on the study of alternative and clean fuels. One of the prospective alternative fuels is natural gas. Methane is the major constituent of natural gas as well as the smallest hydrocarbon fuel. Therefore, methane is a key fuel candidate of research. Methane has been in use on specific combustion devices like internal combustion engines and industrial gas turbines operated at high pressure and temperature.

At room temperature and standard pressure, methane is a colorless, odorless gas. The familiar smell of natural gas as used in homes is achieved by the addition of an odorant, usually blends containing tert-butylthiol, as a safety measure. Methane has a boiling point of 164 C at a pressure of one atmosphere. As a gas it is flammable over a range of concentrations (5.4 to 17%) in air at standard pressure.

Solid methane exists in several modifications. Presently nine are known. Cooling methane at normal pressure results in the formation of methane I. This substance crystallizes in the cubic system. The positions of the hydrogen atoms are not fixed in methane I, i.e. methane molecules may rotate freely. Therefore, it is a plastic crystal.

Combustion of stoichiometric methane mixture in air:

$CH_4 + 2(o_2 + 3.76N_2) \longleftrightarrow CO_2 + 2H_2) + 7.52N_2$

The aim of this simulation is measurement the ignition delay time for a mixture of air and methane as well as how this time depends on quantity of fuel.

2 Description of phenomenon

Ignition delay time is a key parameter of fuel chemistry, which can serve as the validation parameter in the development of chemical kinetics. Shock tube is a standard facility to measure the ignition delay time at high temperatures. It is zero-dimensional and homogeneous inside, so the ignition of fuel oxidizer mixtures is controlled by chemical kinetic. Additionally, shock tube can measure the ignition delay time at the specified pressure and temperature.

Generally ignition delay is the time between fuel injection and fuel ignition. During this time the fuel get mixed with hot compressed air and vaporizes. After the ignition delay, spontaneous ignition of the fuel occurs. The ignition delay time is a readily measurable quantity that is a function of the initial temperature, pressure, and composition of the reactant mixture. For methane, it has been found that the ignition delay time can be correlated in the form:

$t = e^{\frac{E}{RT}}[CH_4]^a[O_2]^b$

where the term E is a parameter equivalent to a global activation energy and A is an empirically determined constant. The terms [CH4] and [Oz] are the molar concentrations (mol/cc) of methane and oxygen, respectively, in the combustible mixture. The empirical exponents a and b of these terms express the power dependencies of ignition delay time on fuel and oxidizer concentrations. The concentrations are determined by

$[]_i = x_i \frac{P}{RT}$

where x is the mole fraction of fuel or oxygen, P is the pressure, T is the temperature of the mixture at the point of ignition and R is the universal gas constant. Correlation of experimental data for methane by means of these equations shows that ignition delay time decreases for both increasing temperature and increasing pressure.

3 Simulation

The simulation was conducted using Cantera, which is a software tool for Python language.

The chemical kinetic model utilized in the study includes GRI Mech 3.0. There are 325 elementary chemical reactions and associated rate coefficient expressions and thermochemical parameters for the 53 species in GRI Mech 3.0. The ranges of its application are 10002500 K in temperature, 10 torr10 atm in pressure and 0.15.0 in equivalence ratio. It includes the detailed combustion reaction mechanism for hydrogen.

3.1 Initial conditions

Temperature was set to $1000K$
Pressure : $1atm$
Mole composition: CH_4: 0,5, O_2: 1, N_2: 3,76

3.2 Calculations

Time range was set to 1,4 s and measurements of temperature and mole fractions $(0_2, CH_4, H)$ were written every 0,005 s. Results are shown after execution of the program. They are too long to put them in the report. Ignition is defined as the moment, when occurs rapid increase of temperature. Plot below points it exactly:

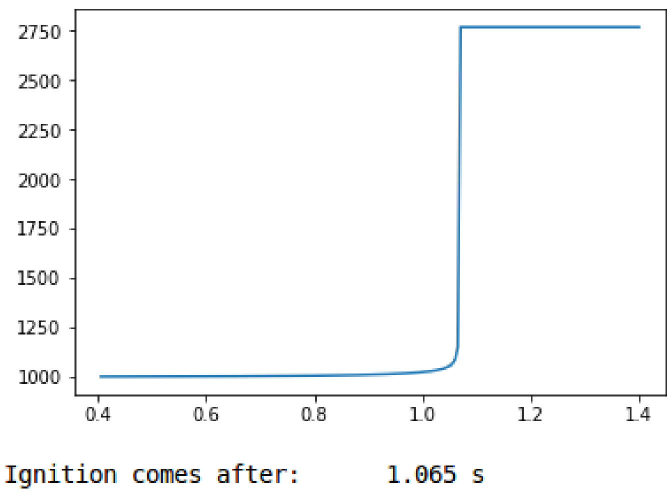
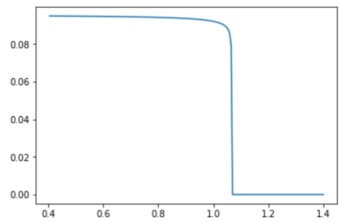
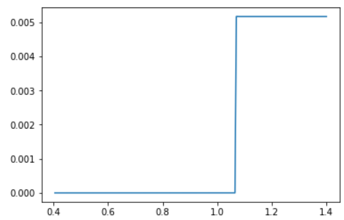


Figure 1: Plot of temperature [K] versus time [s]

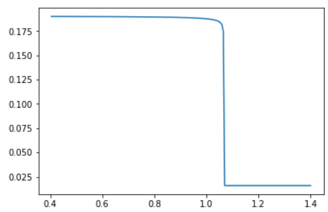
Now let's take a look at plots of mole fractions.



(a) CH_4



(b) H_2



(c) O_2

Figure 2: Plots mole fraction [%] versus time [s]

On figure 2c it is seen that not all of O_2 disappeared. It exists in products too. On the other hand all of H_2 discharged after combustion.

3.3 Additional calculations

Next calculations were conducted to show how quantity of fuel depends on ignition delay. The range for moles of methane was set from 0,1 to 0,8. Initial temperature and pressure remained the same as in above calculations. Below there's a comparison:

CH4 [mole]	Ignition time [s]
0.1	0.550
0.2	0.680
0.3	0.825
0.4	0.950
0.5	1.065
0.6	1.170
0.7	1.270
0.8	1.365

Figure 3: Comparative table

And plot:

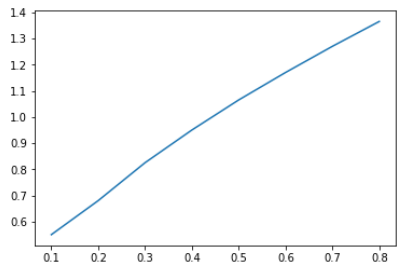


Figure 4: Plot of ignition time [s] versus mole of methane

4 Observation and Conclusion

- Ignition delay time strictly depends on quantity of fuel
- For the same quantity of oxidant if there's more fuel then ignition delay is longer (Only in mentioned conditions - this function is not linear).
- Not all of oxygen is burned.
- All of hydrogen discharged after combustion.
- Ignition delay time is an important parameter in combustion issues.

5 Analised literature

1. Laminar flame speeds and ignition delay times of methaneair mixtures at elevated temperatures and pressures by Erjiang Hu, Yizhen Chen, li Xiaotian, Yongliang Xie
2. Ignition delay characteristics of methane fuels by L. J. Spadaccini and M. B. Colket