Autoignition of hydrogen-air mixtures - numerical simulation on AWS EC2

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1 Introduction

The main purpose of this paper is to present the calculation process fulfilled on AWS (Amazon Web Services) EC2 Linux instance. Conducted numerical calculations concerned adiabatic autoignition process of different hydrogen-air mixtures in constant volume reactor.

2 Virtual computing instance

AWS EC2 Linux instance (Windows client) was used in calculation process. Connection was established via SSH protocol. The result files of the simulation were automatically saved on AWS EC2 and afterwards moved to AWS S3 bucket.

The most challenging part of the project concerned the configuration of cloud computing instance. Configuration process consisted of:

- installation of Anaconda
- adding Cantera package to Anaconda
- configuration of Matplotlib in Anaconda

To achieve compliance with EC2 instance's requirements, customization of Matplotlib's configuration file was necessary.

3 Numerical simulation description

Cantera software

Cantera is a suite of object-oriented software tools for problems involving chemical kinetics, thermodynamics and/or transport processes. Cantera provides types (or classes) of objects representing phases of matter, interfaces between these phases, reaction managers, time-dependent reactor networks and steady one-dimensional reacting flows. Cantera is currently used for applications including combustion, detonations, electrochemical energy conversion and storage, fuel cells, batteries, aqueous electrolyte solutions, plasmas, and thin film deposition.

Cantera allows also simulating processes taking place in reactors and combustion chambers.

In this project Cantera2.3.0 was used from Python. In addition, Matplotlib was used to graphically present obtained results.

Simulation concerns constant volume reactor in which homogeneous hydrogen-air mixture is exposed on temperature $1000K$, which leads to its autoignition. Numerical method was tested for variety values of hydrogen percentage in the mixture and different initial pressure values.

Range of hydrogen percentage in the mixture: **4% - 74,5%**, step: 0,5%.
Range of pressure: **0,2 atm - 1,5 atm**, step: 0,1 atm

Cantera software gives an ability to simulate this autoignition process and generate the temperature history as a function of time. It also enables to estimate the ignition temperature and delay time.

Parameters history was generated with 0,00001 s time step from $t_0 = 0$ to $t_{end} = 0,001s$

Numerical code in Cantera (Python) can be found on GitHub (https://github.com/jwadolowska/CloudComputing).

4 Results

The result of the experiment is value of autoignition temperature and delay time for combustible mixtures with different hydrogen contents exposed to different initial pressures.

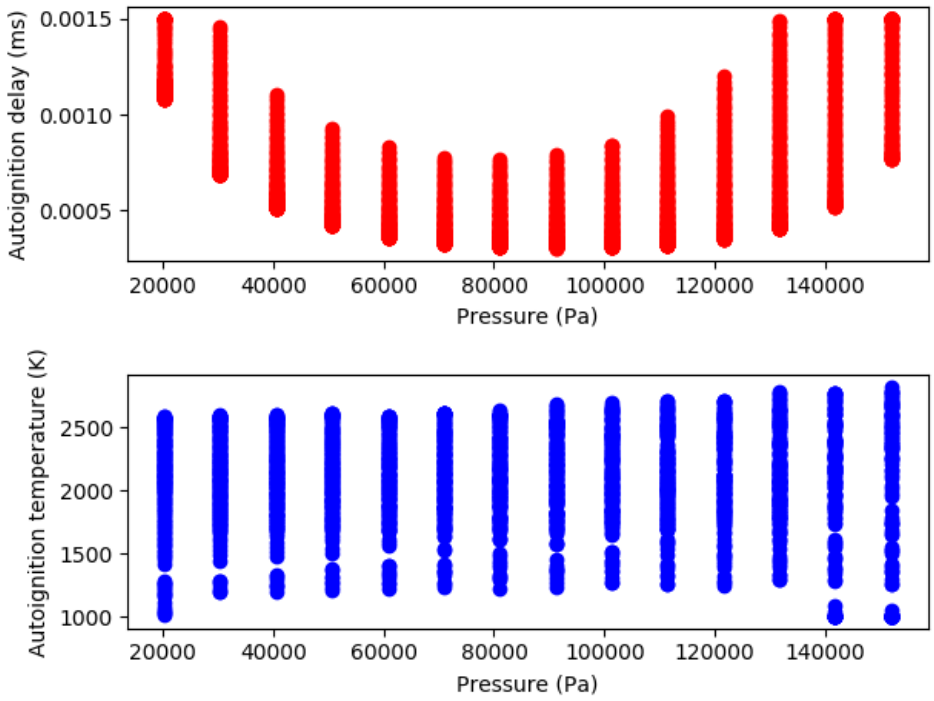

Figure 1: Dependence of the autoignition temperature on the mixture's composition and initial pressure.

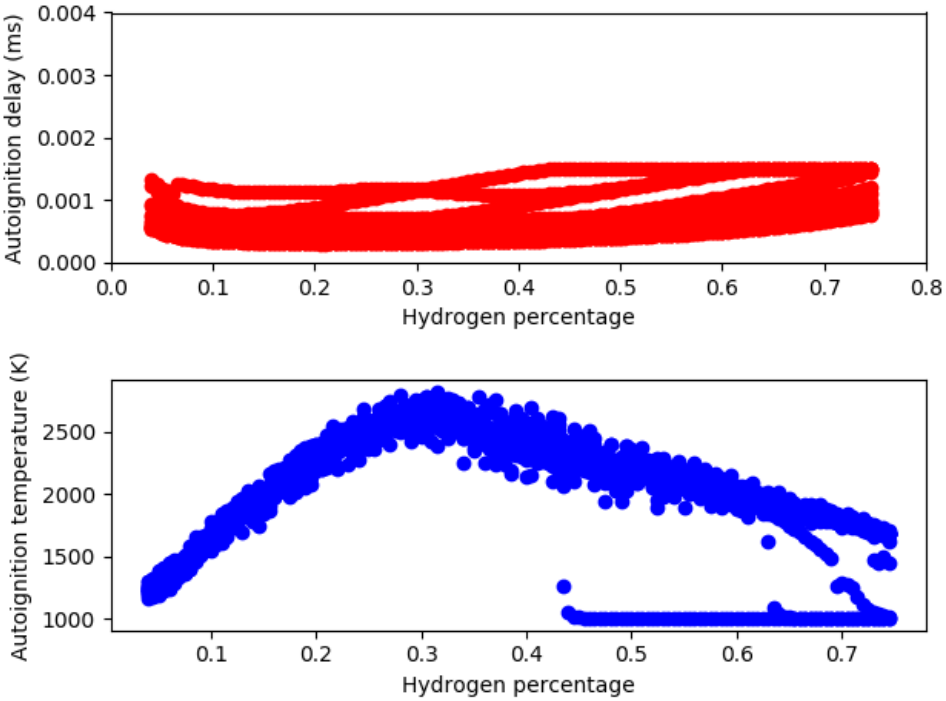

Figure 2: Dependence of the ignition delay time on the mixture's composition and initial pressure.

5 Summary

AWS, as a very powerful computation service, can be used to help faster obtain results of many numerical simulations and much faster solve number of engineering problems.

It can be easily noticed, that presented diagrams generated as a result of presented simulation consists of too many points, what makes them indistinct. Obtained results can be presented better using .txt files generated along the diagrams.