Metody komputerowe w spalaniu

Investigation of Chapman–Jouguet Detonation Parameters for Different Mixtures

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Spis treści

1. Introduction

The study of **detonation phenomena** is a critical area within combustion science, with applications ranging from propulsion systems to explosion safety. One of the foundational theoretical frameworks for describing detonation waves is the **Chapman–Jouguet (CJ) theory**, which defines the conditions under which a detonation wave propagates at a steady state. According to CJ theory, a detonation wave consists of a leading shock wave followed by a zone of chemical reaction, terminating where the flow velocity relative to the shock front equals the local sound speed of the products.

In this report, we investigate the CJ detonation parameters for several fuel-oxidizer mixtures using Python and the **Cantera** library, a powerful chemical kinetics and thermodynamics package developed by the *Explosion Dynamics Laboratory at Caltech*. This computational approach allows precise simulation of complex reaction mechanisms and thermodynamic properties of reacting flows.

The mixtures examined in this study include:

- Hydrogen and oxygen: $H_2 + O_2$
- Methane and oxygen: $CH_4 + O_2$
- Acetylene and oxygen: $C_2H_2 + O_2$
- Hydrogen and air (approximately $H_2 + (O_2 + 3.76N_2)$)
- Methane and air (approximately $CH_4 + (O_2 + 3.76N_2)$)

Each of these mixtures presents distinct characteristics in terms of flame speed, ignition delay, and detonation velocity. For example, hydrogen–oxygen mixtures are known for their high reactivity and low ignition energy, while methane–air mixtures represent more practical, but less sensitive fuels.

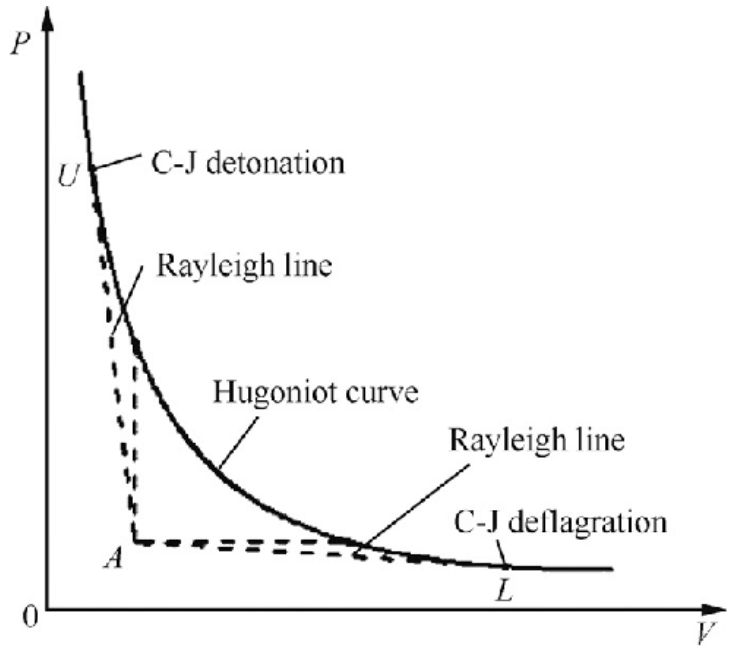
The objective of this study is to compute key CJ detonation parameters, including:

- CJ detonation velocity
- local sound velocity
- Post-detonation pressure and temperature
- Final composition of reaction products
- Final local density

2. Problem describtion and Theory behind It

The Chapman–Jouguet (CJ) theory provides a simplified but powerful model for describing detonation waves in reactive gas mixtures. In this theory, a detonation is idealized as a one-dimensional wave consisting of a leading shock wave followed by instantaneous chemical reaction. The key feature is the **CJ point**, which represents the thermodynamic state of the detonation products where the flow relative to the detonation front becomes

sonic. This condition ensures that no information can propagate upstream to affect the detonation front, making the wave self-sustaining.



Rysunek 2.1. Classic CJ detonation diagram showing the Rayleigh line, Hugoniot curve, and the Chapman–Jouguet point in the pressure–specific volume (p–v) plane.

In the CJ model, the conservation laws of mass, momentum, and energy are applied across the detonation front. Assuming a steady, planar detonation, and using a control volume fixed to the shock, the governing equations are:

$$\rho_1 u_1 = \rho_2 u_2 \qquad \text{(mass conservation)} \tag{1}$$

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \qquad \text{(momentum conservation)} \tag{2}$$

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2} \qquad \text{(energy conservation)} \tag{3}$$

where subscripts 1 and 2 refer to the unburned and burned gas states, respectively, ρ is the density, u is the velocity in the shock-fixed frame, p is the pressure, and h is the specific enthalpy.

The detonation velocity at the CJ point, U_{CJ}, is the minimum velocity at which a stable detonation can occur. The strong leading shock wave rapidly compresses the unreacted mixture, increasing its temperature and pressure. This is followed by rapid exothermic reactions, which further increase the internal energy of the mixture.

Behind the shock front, the pressure and temperature rise sharply. The pressure increase is much higher than in subsonic deflagration processes and can be several times the initial pressure. The flow is choked at the CJ point, where the burned gases exit the

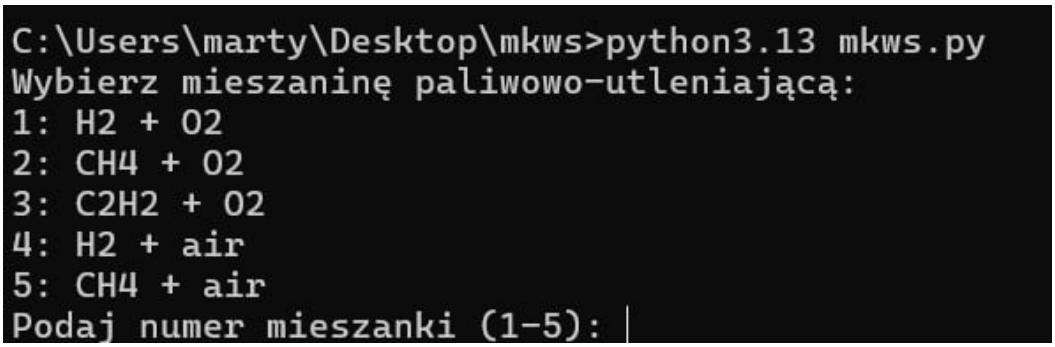
reaction zone at the local speed of sound relative to the shock frame:

$$u_2 = c_2$$

This sonic condition is essential for defining the CJ detonation, as it imposes a unique solution to the Rankine–Hugoniot equations.

3. Program structure

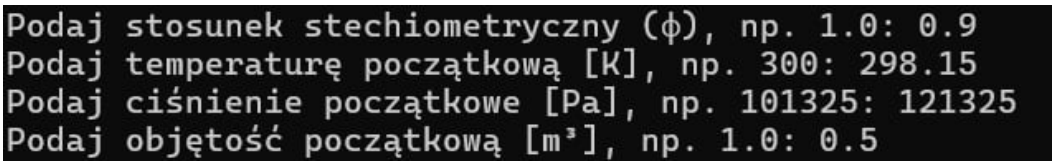
Program allows to choose one out of five different mixtures, the flow of it will be shown below:



Rysunek 3.1. 1st step, choosing a miture

After that, the usage of code is based on providing it with 4 parameters, as follows:

- stechiometry coefficient ϕ
- initial temperature T_0
- initial pressure p_0
- initial volume V_0



Rysunek 3.2. 2nd step. including 4 parameters

The computational analysis in this study uses the **Cantera** library—an open-source suite for solving problems involving chemical kinetics, thermodynamic properties, and transport processes.

Cantera solves the fundamental conservation equations for a reacting system. For a closed homogeneous reactor at constant internal energy and volume (isochoric and adiabatic conditions), the governing equations are derived from:

- **Mass conservation for species** k:

$$\frac{dY_k}{dt} = \frac{\dot{\omega}_k M_k}{\rho}$$

  where Y_k is the mass fraction, $\dot{\omega}_k$ is the molar production rate, M_k is the molar mass, and ρ is the mixture density.
- **Energy conservation (internal energy form)**:

$$\frac{du}{dt} = -\frac{p}{\rho^2}\frac{d\rho}{dt} + \sum_k h_k \frac{dY_k}{dt}$$

  or under constant volume:

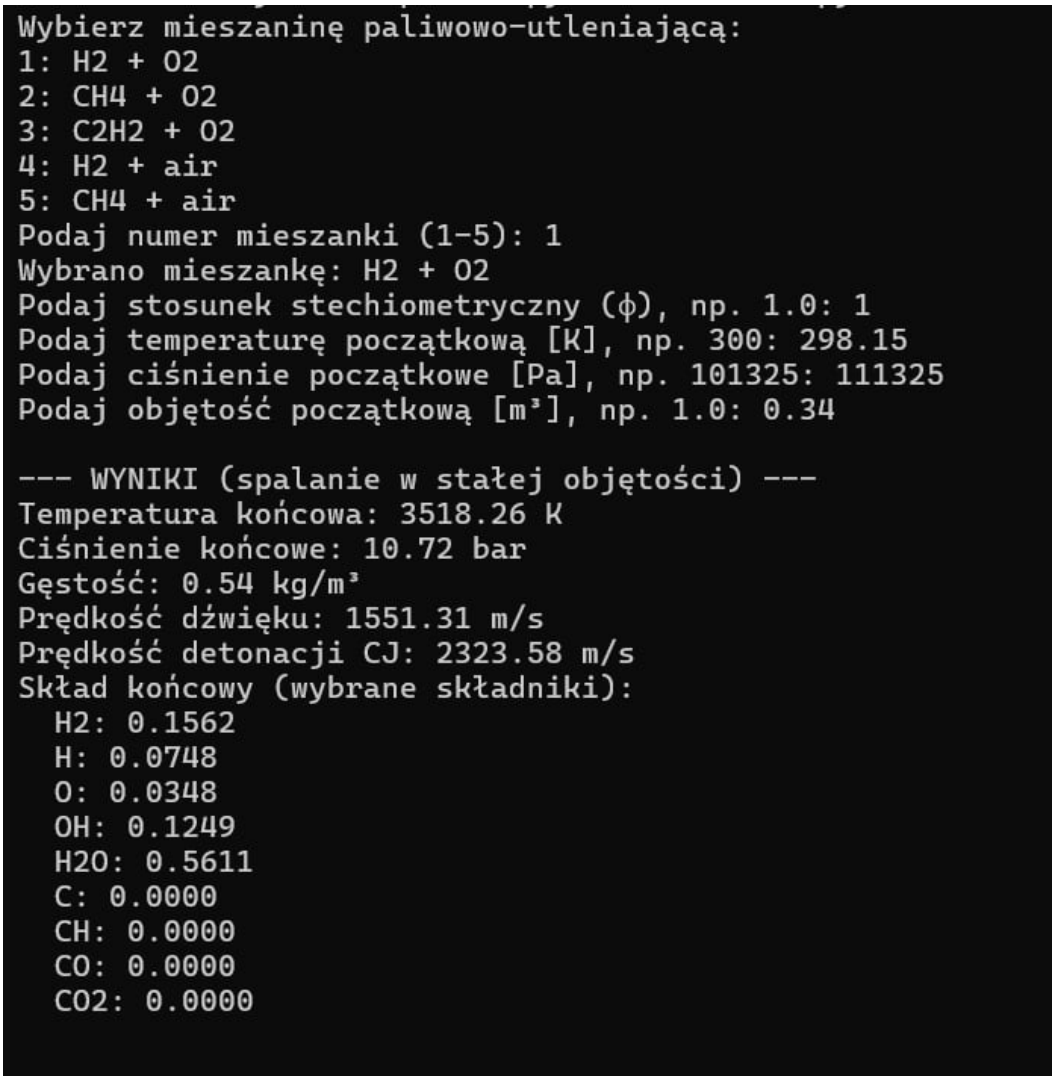
$$\frac{dT}{dt} = \frac{-1}{\rho c_v}\sum_k h_k \dot{\omega}_k M_k$$

  where c_v is the specific heat at constant volume, and h_k is the specific enthalpy of species k.
- **Equation of state (ideal gas)**:

$$p = \rho R T = \rho \left(\frac{R_u}{\bar{M}}\right) T$$

  where R is the specific gas constant, R_u is the universal gas constant, and $\bar{M}$ is the mean molar mass of the mixture.

The CJ detonation velocity is computed using the Rankine–Hugoniot relations combined with thermodynamic equilibrium constraints. The function `CJspeed()` from the `sdtoolbox` package determines the minimum detonation velocity at which the flow becomes sonic relative to the wave front. Cantera handles both the chemical mechanism and the numerical integration of stiff systems of differential equations, making it suitable for accurate prediction of post-detonation states, species composition, and sound speed.

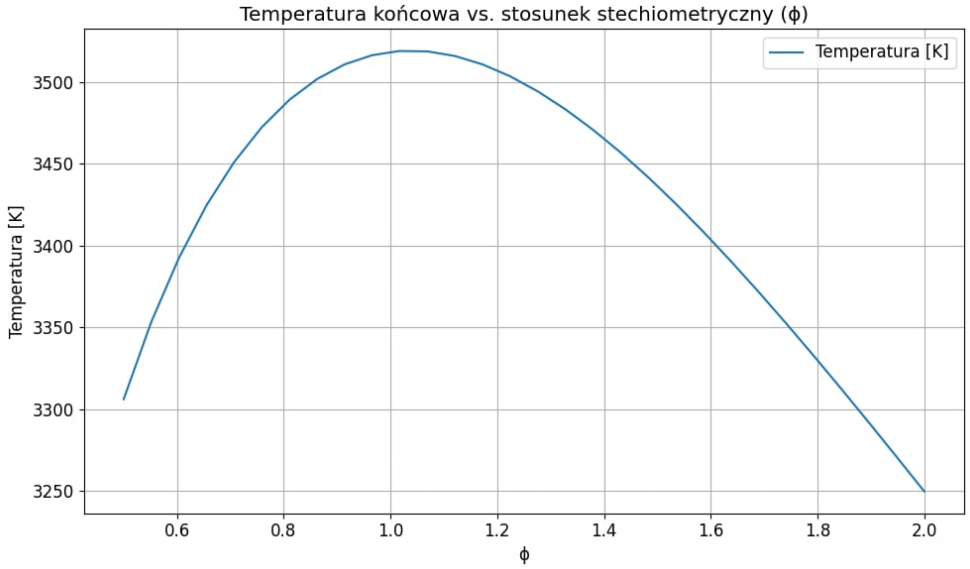


Rysunek 4.1. Output of the program showing thermodynamic and detonation parameters for the selected mixture.

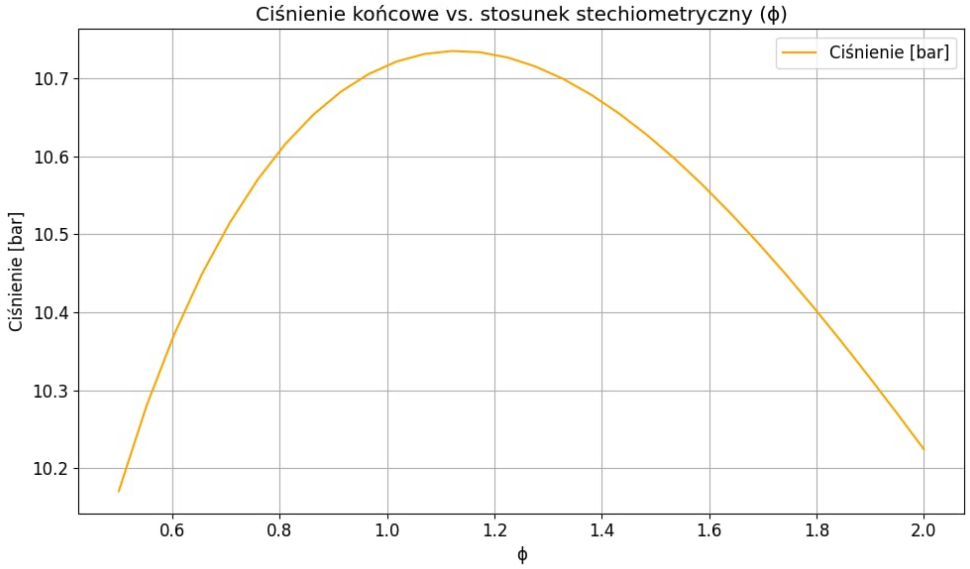
4. Results

The results generated by the simulation program are presented below. Figure 4.1 shows the printed output from the Cantera-based code, including calculated values such as final temperature, pressure, density, speed of sound, CJ detonation velocity, and selected species concentrations.

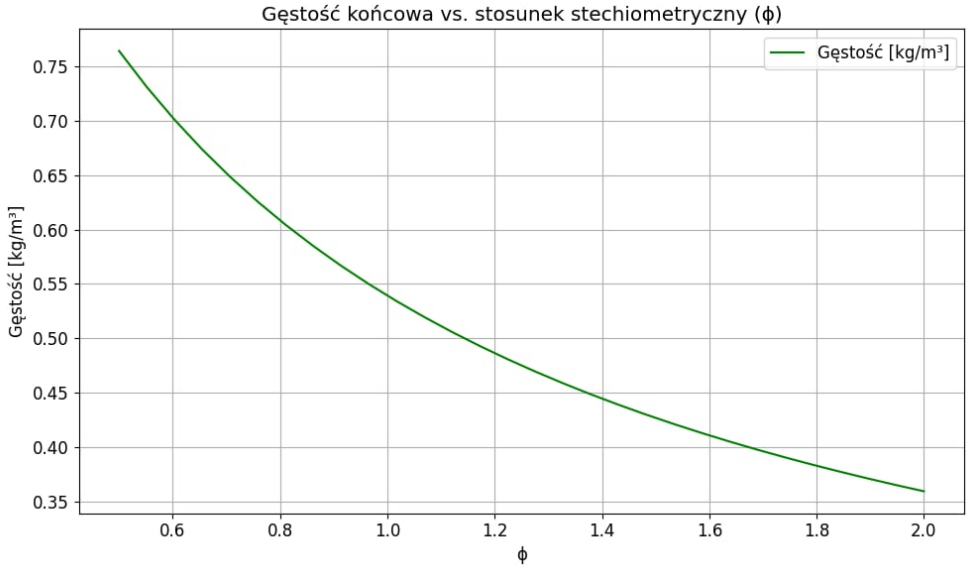
A plot of final temperature, pressure, density and products of reaction as a function of equivalence ratio (ϕ) is presented below. This diagrams illustrate how mixture richness influences the thermal state of the combustion products under constant-volume equilibrium conditions.



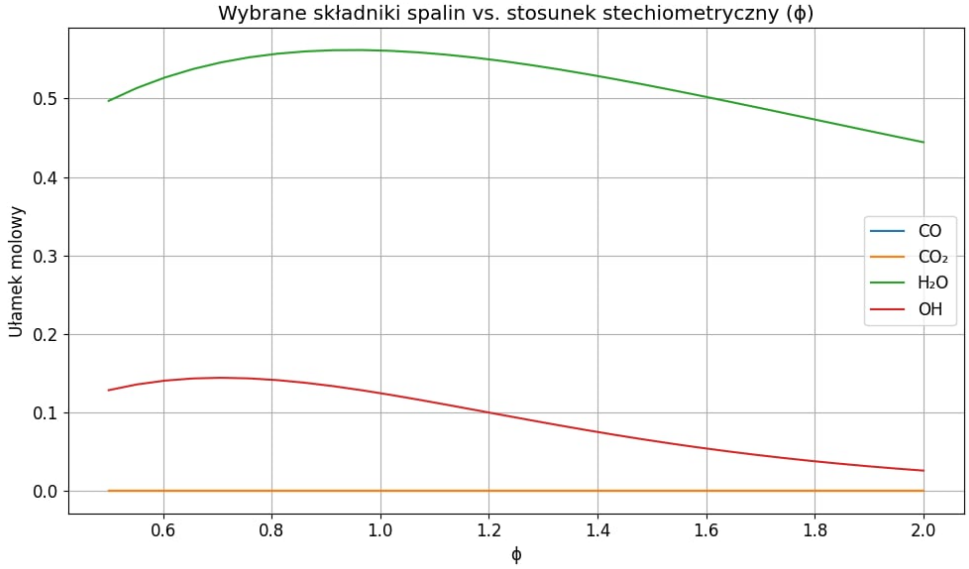
Rysunek 4.2. Final temperature vs. equivalence ratio ϕ for a selected fuel-oxidizer mixture.



Rysunek 4.3. Final pressure vs. equivalence ratio ϕ for a selected fuel-oxidizer mixture.



Rysunek 4.4. density vs. equivalence ratio ϕ for a selected fuel-oxidizer mixture.



Rysunek 4.5. reaction products vs. equivalence ratio ϕ for a selected fuel-oxidizer mixture.

5. Summary

The presented numerical approach, based on the Cantera library and equilibrium combustion analysis, offers a quick and accurate method for estimating key detonation parameters. The ability to compute final thermodynamic states, species concentrations, and the CJ detonation velocity for various fuel-oxidizer mixtures allows for rapid assessment of detonation behavior under different initial conditions. Despite certain idealizations—such as instantaneous chemical equilibrium and neglect of finite reaction zone structure—the method provides a reliable first-order approximation. As such, it serves as a robust foundation for more detailed modeling or experimental validation in advanced detonation research and engineering applications.

6. Sources

1. Cantera Mechanism Files – Caltech EDL
2. S. Wójcicki *Spalanie*