Faculty of Power and Aeronautical Engineering
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Computer Methods in Combustion

Parameters of Chapman-Jouguet detonation of methane-air and hydrogen-air mixtures

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1. Introduction

Chapman-Jouguet (CJ) detonation is a fundamental phenomenon in the field of combustion, characterized by the self-sustaining propagation of a shock wave through a reactive mixture at a steady-state condition. Understanding the parameters governing Chapman-Jouguet detonation is crucial for predicting and controlling combustion processes in various engineering applications. While extensive research has been conducted on the detonation characteristics of hydrocarbon-air mixtures, there is a need to investigate the specific parameters associated with methane-air and hydrogen-air mixtures. Methane, as the primary component of natural gas, is an important fuel source and understanding its detonation properties is vital for safety considerations in energy production and transportation systems. Hydrogen, on the other hand, is gaining attention as a clean energy carrier, and exploring the detonation characteristics of hydrogen-air mixtures is essential for ensuring the safe implementation of hydrogen-based technologies. Therefore, this study aims to investigate the parameters of Chapman-Jouguet detonation for methane-air and hydrogen-air mixtures, providing valuable insights into the combustion behavior of these important fuel systems.

2. Literature overview and theoretical background

2.1. Governing equations for a combustion wave in a premixed gas

Imagine a long tube closed at both ends and filled with combustible gas mixture. Now take away both ends cover rapidly and ignite the gas at one end. We will see a combustion wave propagating down the tube with constant speed of less than one meter per second. If we now repeat the experiment and only take away one cover and ignite the gas at the other end, a combustion wave starts to propagate with the same speed as in the first case but in a short while we obtain a combustion wave that propagates at a velocity several times the speed of sound of the unburned gas. If we take away the remaining cover, the wave will continue to propagate at supersonic speed. In the first case we have a deflagration wave and in the latter a detonation wave.

Consider a mixture of combustible gases in a straight pipe of constant cross section in which we have a plane combustion wave propagating along the pipe axes. The wave is described in coordinate system stationary to the wave.

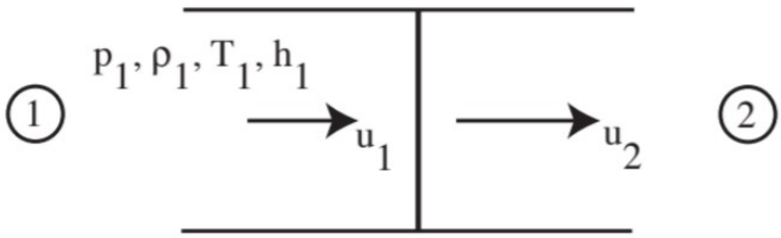


Figure 2.1. One dimensional wave propagation inside the conduit (pipe)

The governing equations preserving mass, momentum and energy are:

$$\rho_1 u_1 = \rho_2 u_2 = \dot{m_{au}}$$
$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2$$
$$h_1(T_1) + \frac{1}{2}u_1^2 = h_2(T_2) + \frac{1}{2}u_2^2$$

where $\dot{m_{au}}$ is the mass flux per area unit. In addition, we have the ideal gas law:

$$p = \rho R T$$

where R is the specific gas constant (with index 1 or 2 for the inlet and outlet gases respectively). The enthalpy is given as:

$$h(T)_j = \left[\sum_i Y_i h_f\left(T_{ref}\right) + \int_{T_{ref}}^{T} c_p dT\right]_j$$

where j is either 1 or 2 indicating the side of the wave.

If we now look at the combustion wave problem we neither know the velocity of the inlet and outlet gas nor the combustion products. In all we have 5 unknown u_1, u_2, p_2, ρ_2 and T_2 but only 4 equations. The fifth equation relates the composition of the combustion products with the temperature T_2 and total pressure p_2 which could be determined in an equilibrium situation. However a great deal of insight into the problem is gained plotting the relation between pressure and density over the wave both as a function of the mass flux (Rayleigh line) and the heat release, q (Rankine-Hugoniot relation).

We start out with equations preserving mass and momentum slightly rewritten in the following ways:

$$\left(\rho_1 u_1\right)^2 = \left(\rho_2 u_2\right)^2 = (\dot{m_{au}})^2$$
$$p_2 - p_1 = \frac{\rho_1^2 u_1^2}{\rho_1} - \frac{\rho_2^2 u_2^2}{\rho_2}$$

Eliminating the velocity we get

$$p_2 - p_1 = (\dot{m_{au}})^2 \left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right)$$

Thus from the inlet conditions at 1 we have our outlet condition somewhere along line. This is a straight line in a $\left(\mathrm{p}, \frac{1}{\rho}\right)$ diagram always with a negative slope, also called **the Rayleigh line**.

Also by transforming equation of mass, momentum and energy preservation we can obtain:

$$\frac{\kappa}{\kappa - 1}\left(\frac{p_2}{\rho_2} - \frac{p_1}{\rho_1}\right) - \frac{1}{2}\left(\frac{1}{\rho_1} + \frac{1}{\rho_2}\right)\left(p_2 - p_1\right) = q$$

This equation is referred to as the **Rankine-Huginot relation**. In the case of $q = 0$ this is recognized as the Hugoniot relation for a shock.

2.2. Rankine-Hugoniot curve

Drawing the Rankine-Hugoniot (R-H) curve and the Rayleigh line in the same diagram, gives us the visual aid to discuss where a solution to the equations is to be found. Figure 2.2 shows the R-H curve and Rayleigh line in a normalized $\frac{p}{p_1} - \frac{\rho_1}{\rho}$ diagram with the inlet condition at $(1,1)$. The curve drawn with a full line is the $\mathrm{R-H}$ curve for q > 0, whereas the dash-dot line shows the case when q = 0, i.e. the shock Hugoniot curve. The full straight lines are Rayleigh lines for a few different mass fluxes. Now the solutions, the outlet conditions, are found at the intersection of the Rayleigh line and the $\mathrm{R-H}$ curve.

To discuss the matter we have divided the $\mathrm{R-H}$ curve into five segments, $\mathrm{I-V}$.

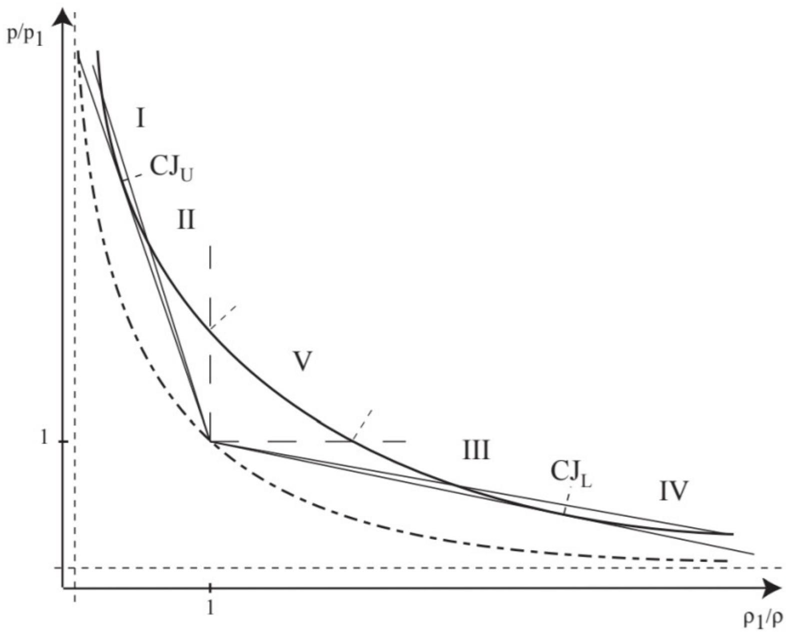


Figure 2.2. Rankine-Hugoniot curve and Rayleigh line. Straight lines are Rayleigh lines for different massfluxes. The dash-dot curve is the shock Hugoniot curve.

Region I **(strong detonation)** is from the highest output pressure to the point on the R-H curve where the Rayleigh line touches it, the so called upper ChapmanJouguet point, CJU.

Region II **(weak detonation)** extends from CJU to where the vertical dashed line crosses the R – H curve.

Region V is the next part and covers the curve down to where the horizontal dashed line intersects the R-H curve.

Region III **(weak deflagration)** covers the part of the curve down to where the Rayleigh line is tangent to the R – H curve, the lower Chapman-Jouguet point, CJL.

Region IV **(strong deflagration)** covers the R – H curve to the right of CJL.

The different regions are called, based on the pressure change over the wave. The inlet Mach number, M1, is positive. We directly see that the slope of the Rayleigh line has to be negative and thus region V is not a physical solution.

2.3. Internal structure of a plane detonation wave. The ZND theory (Zeldovich, Neumann, Döring

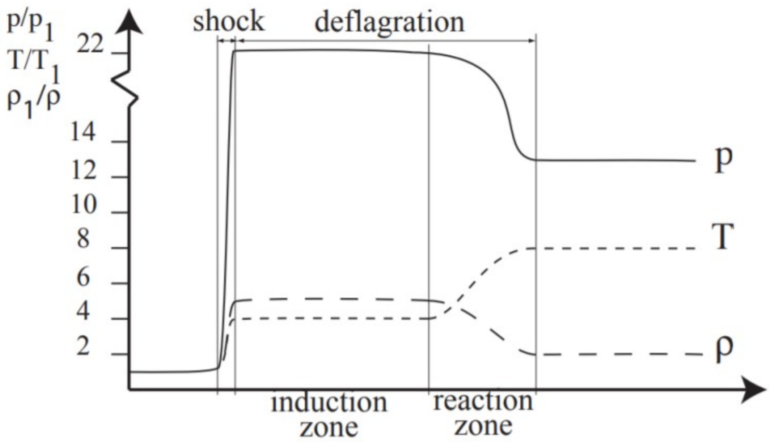


Figure 2.3. ZND wave

The detonation wave although it may appear plane, it is not. Experiments show that wave front consists of both waves moving in the main propagation direction and in spanwise direction and that the front has triple points (three shocks meeting in a point) moving in spanwise direction. However the assumption that the detonation wave essentially consists of a shock wave followed by a deflagration zone, the so called ZND detonation wave, gives a good description and quantitatively correct results for the Chapman-Jouguet detonation. The internal structure is made up of a shock, a few mean free paths thick, where the pressure rises drastically, usually more than 20 times, and temperature and density to more moderate levels i.e. 4-6 times. The shock is followed by a much thicker induction zone where the state variables are almost constant, the chemical reaction starts but does not come to full rate and finally a reaction zone where density and pressure decrease by a factor of about two, while the temperature rises by a similar factor. A schematic of the internal structure is depicted in figure 2.3

2.4. Approximate determination of the Chapman-Jouget detonation velocity

The $C-J$ detonation is very special as the outlet gas velocity is sonic and downstream expansion waves will not catch up with the wave and weaken its strength. Experimentally it is found that free running detonations are often C-J detonations and it is therefore of interest to calculate its characteristics as the detonation velocity and the change in pressure, temperature and density over the wave. An analytical solution is not possible, but with some approximations we get an estimate of the outlet condition.

Assuming constant heat capacities of the reactants and transforming mass, momentum and energy conservation equations with $u_2^2 = a_2^2 = \kappa_2 R_2 T_2 = \kappa_{\rho_2}$ we can finally obtain:

$$u_{CJ} = \sqrt{2\left(\kappa_2^2 - 1\right)\left(q + c_{p_1} T_1\right)}$$

3. Methodology

3.1. Experimental setup

The experimental methodology involves utilizing computational simulations to calculate the Chapman-Jouguet (CJ) detonation speeds of methane-air and hydrogen-air mixtures. The simulations are performed using the Cantera software package, which provides a robust platform for modeling reactive flows and analyzing the thermodynamic and chemical properties of various fuel-air mixtures. The specific steps involved in the methodology are outlined below.

3.2. Computational simulations

To begin, the Cantera package is imported along with other necessary libraries such as NumPy, matplotlib, and sdtoolbox. These libraries enable efficient numerical computations, plotting of results, and access to post-shock calculations for the CJ detonation speed determination.

3.3. Calculations of CJ speed

The CJ speed is calculated for a range of pressure and temperature conditions. Initially, the input parameters such as initial pressure (P1), maximum pressure (Pmax), initial temperature (T1), maximum temperature (Tmax), number of pressure steps (p_steps), number of temperature steps (T_steps), fuel-air composition (q), and the mechanism file (mech) are defined. The fuel-air compositions considered are:

1. **Methane-Air**
   a) lean: CH4:0.5 O2:2.0 N2:7.52
   b) slightly lean: CH4:0.75 O2:2.0 N2:7.52
   c) stoichiometric ratio: CH4:1.0 O2:2.0 N2:7.52
   d) slightly rich CH4:1.5 O2:2.0 N2:7.52 *
   e) rich: CH4:2.0 O2:2.0 N2:7.52
2. **Hydrogen-Air**
   a) lean: H2:1.0 O2:1.0 N2:3.76
   b) slightly lean: H2:1.5 O2:1.0 N2:3.76
   c) stoichiometric ratio: H2:2.0 O2:1.0 N2:3.76
   d) slightly rich H2:3.0 O2:1.0 N2:3.76 *

e) rich H2:4.0 O2:1.0 N2:3.76

Each number represents number of moles of corresponding substance.

A list of arguments is generated, containing combinations of pressure and temperature values based on the specified range and step sizes. This list is used to create a multiprocessing pool, which allows for parallel computation of CJ speeds for different parameter sets.

The calculate_cj_speed function is defined, which takes a set of parameters (pressure, temperature, fuel-air composition, and mechanism file) as input. Within this function, the Cantera Solution object is initialized with the specified mechanism file, and the temperature, pressure, and composition are set. The CJspeed function from the sdtoolbox module is then called to calculate the CJ speed for the given parameters.

The multiprocessing pool is utilized to map the calculate_cj_speed function to the list of arguments, resulting in the computation of CJ speeds for all parameter combinations in parallel to allow for better usage of CPU an therfore to allow faster execution of the calculations. The obtained CJ speeds are stored in a numpy array, which is reshaped to match the specified number of pressure and temperature steps.

3.4. Visualisation

Once the CJ speeds are computed, they are displayed in the console output. Additionally, two sets of plots are generated to visualize the relationship between CJ detonation speed and pressure, as well as CJ detonation speed and temperature. The plots are created using matplotlib, with appropriate labels, titles, and legends to provide clear visual representations of the results.

For each fuel-air mixture (methane-air and hydrogen-air), separate plots are generated for pressure and temperature variations. The CJ speeds corresponding to different temperature or pressure values are plotted against the respective parameter, allowing for a comprehensive analysis of the detonation behavior.

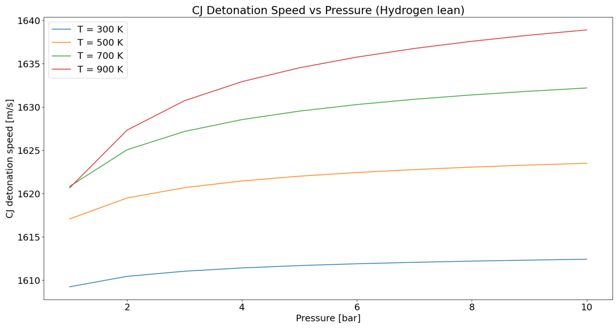
3.5. Data Analysis and interpretation

The obtained CJ speeds for methane-air and hydrogen-air mixtures are examined and analyzed to identify trends and patterns. The effects of pressure and temperature on the CJ speed are evaluated based on the generated plots. The data can be further processed and compared to experimental or theoretical values available in the literature to validate the computational results.

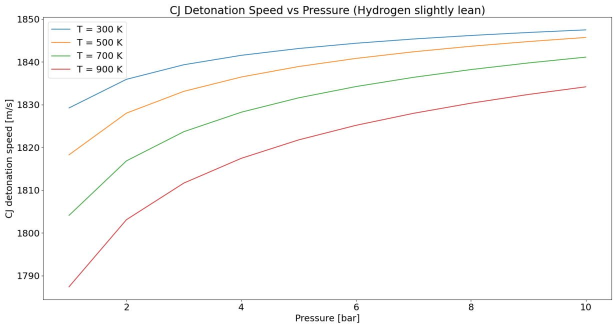
By conducting these computational simulations and analyzing the resulting CJ speeds, valuable insights into the detonation characteristics of methane-air and hydrogen-air mixtures can be obtained. These insights can contribute to the understanding of combustion behavior and aid in the development of improved combustion systems and safety measures.

4. Results and discussion

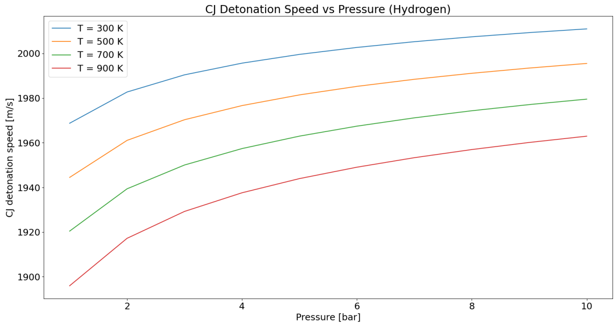
4.1. Hydrogen-Air mixture pressure diagrams



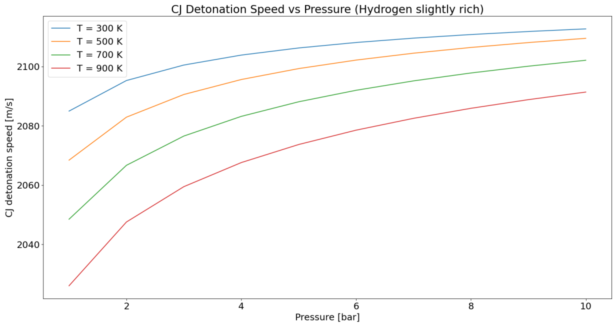
(a) Lean



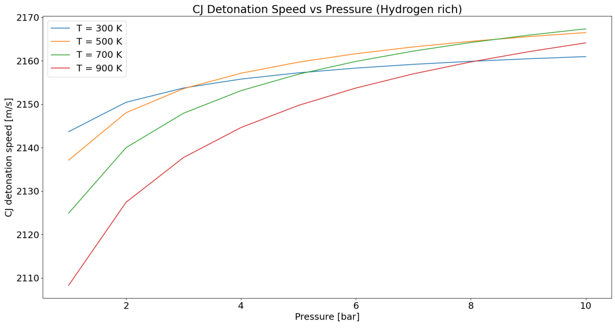
(b) Slightly lean



(c) Stoichiometric



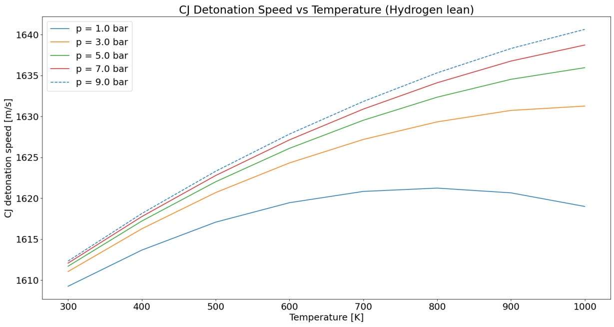
(d) Slightly rich



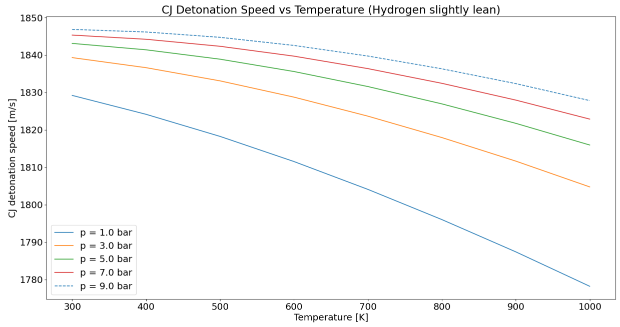
(e) Rich

Figure 4.1

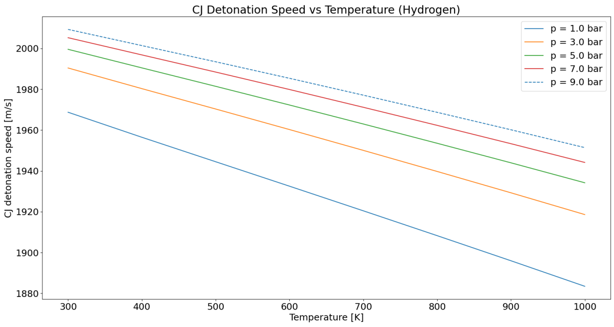
4.2. Hydrogen-Air mixture temperature diagrams



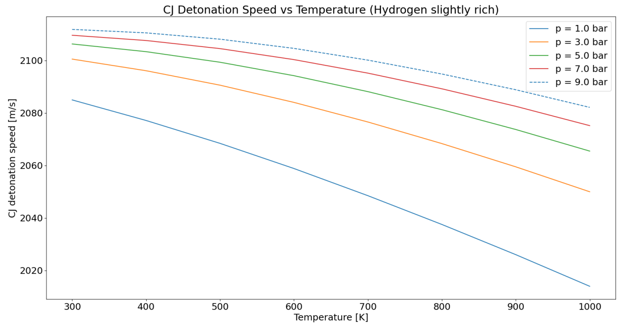
(a) Lean



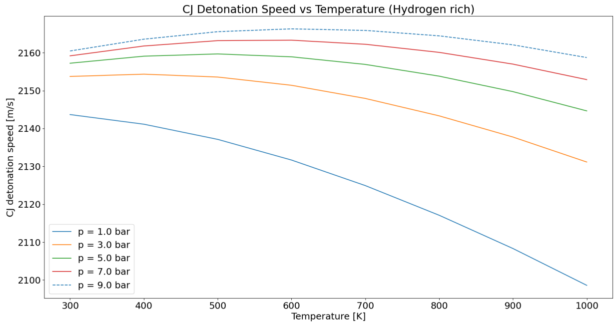
(b) Slightly lean



(c) Stoichiometric



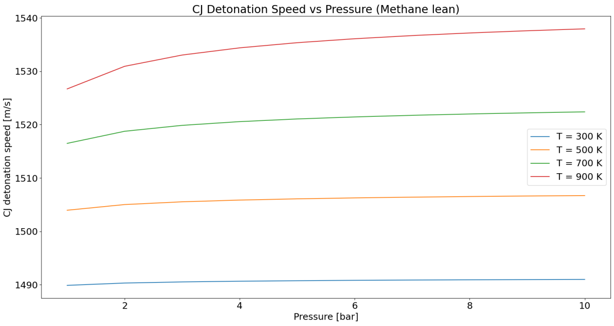
(d) Slightly rich



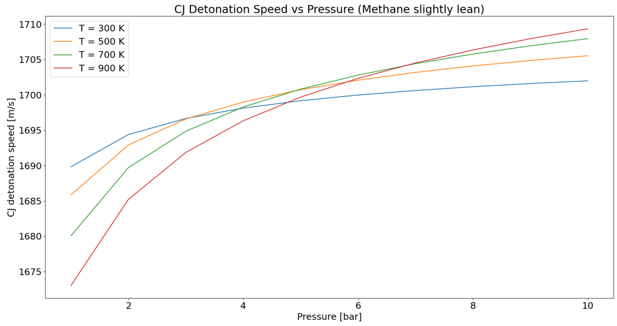
(e) Rich

Figure 4.2

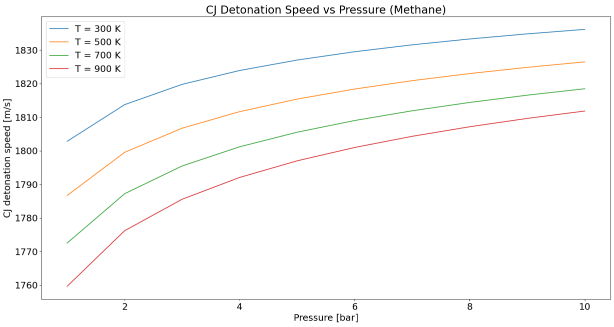
4.3. Methane-Air mixture pressure diagrams



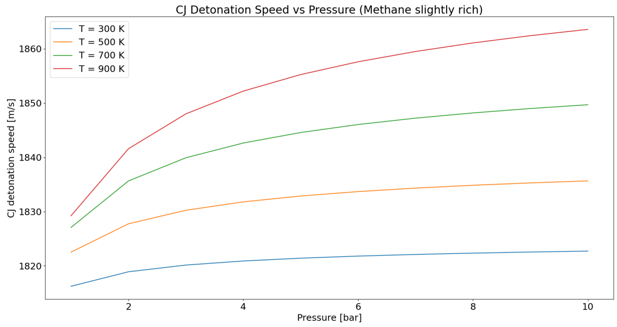
(a) Lean



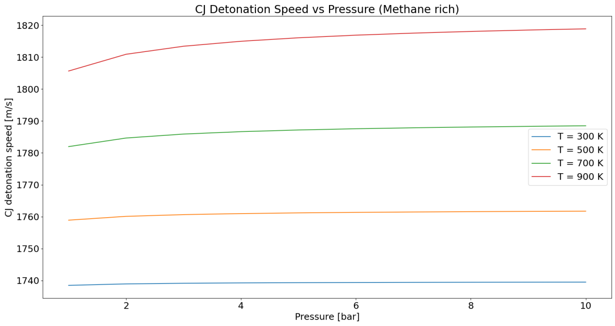
(b) Slightly lean



(c) Stoichiometric



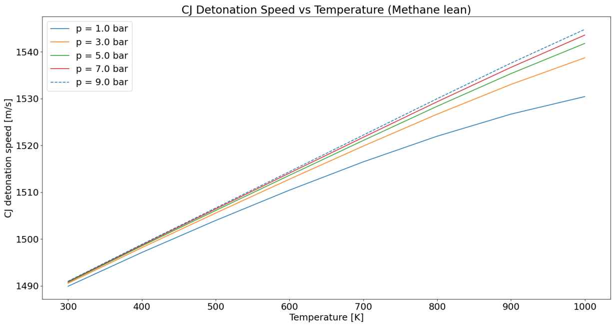
(d) Slightly rich



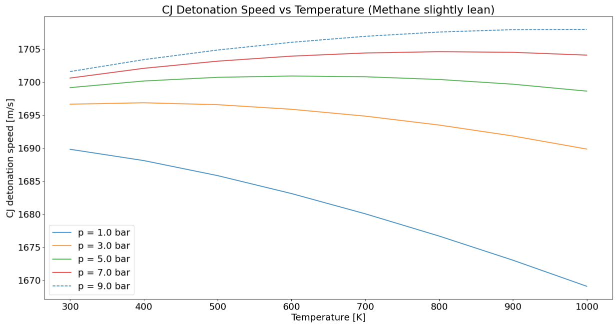
(e) Rich

Figure 4.3

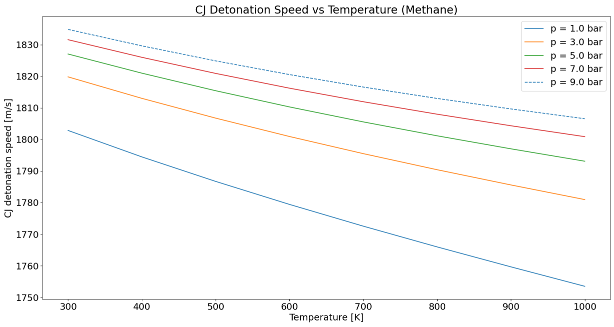
4.4. Methane-Air mixture temperature diagrams



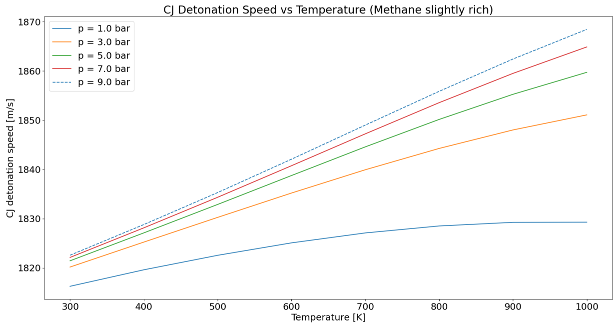
(a) Lean



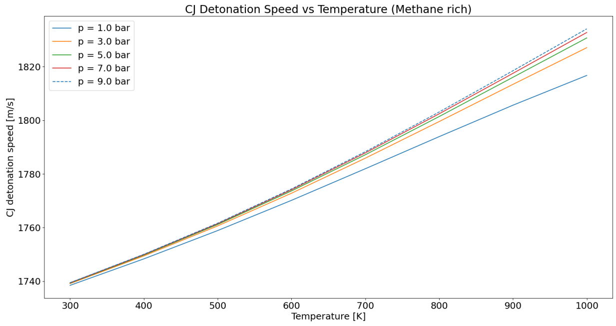
(b) Slightly lean



(c) Stoichiometric



(d) Slightly rich



(e) Rich

Figure 4.4

4.5. Discussion

Analysing CJ detonation speed vs pressure plots for hydrogen (subsection: 4.1) we can see that richer mixtures (more fuel) have higher detonation velocities. The difference between 2 extreme cases (lean vs rich for 10 bar of starting pressure) is almost $500\frac{m}{s}$, whereas the difference between the lowest and highest velocity values in each plot is significantly smaller ($25 < v_{cj} < 100\frac{m}{s}$).With the increase in initial pressure comes the increase of detonation velocity. What is more, in most cases the higher the starting temperature the lower the detonation speeds (with the exception being the rich mixture where, for higher pressures, this trend is reversed).

Analysing CJ detonation speed vs temperature plots for the same mixtures (subsection: 4.2) we can see that in cases excluding the lean mixture (and lower starting temperatures of rich mixture - where the trend is reversed), the higher the temperature the lower the speed of detonation, which is in accordance with previous the analysis.

Analysing CJ detonation speed vs pressure plots for methane (subsection: 4.3),at first glance, it can be noticed that, similarly to hydrogen mixtures, higher starting pressure results in higher detonation velocity but the difference in speeds for each mixture is insignificant compared to the speed difference obtained by change in AF ratio. Upon further inspection, the temperature factor does not appear to follow any clear trend as with different AF ratios the plots seem to be vastly different. Between the stoichiometric and slightly rich ratio there seems to be an inversion in trend. For the stoichiometric ratio lower initial temperature results in higher detonation speeds, for slightly rich ratio it is the opposite.

It can also be noted that rich mixture does not yield the highest speed, which is obtained during detonation of slightly rich mixture.

5. Conclusions

1. Difference in fuel to air ratios are far more impactful on the velocity of detonation than initial pressure or temperature.
2. Richer mixtures (higher fuel-to-air ratios) result in higher detonation velocities. This is consistent with the increased availability of fuel, leading to a more rapid combustion process. With the exception being rich mixture of methane, whic most likely was too rich and too close to the upper flammability limit.
3. Increasing the initial pressure leads to an increase in the detonation velocity. This can be attributed to the enhanced compression and higher reactant concentrations at higher pressures, promoting faster combustion.
4. Except for the lean mixture, higher temperatures are associated with lower detonation

speeds. This inverse relationship suggests that the rate of reaction decreases with increasing temperature for hydrogen-air mixtures.

Based on these observations, we can conclude that the fuel-to-air ratio has a significant influence on the detonation speed of both hydrogen and methane mixtures. Additionally, pressure and temperature also play important roles, but their effects can be modulated by the specific fuel-to-air ratio. These findings highlight the need for a comprehensive understanding of the chemical kinetics and thermodynamics of combustion processes to accurately predict and control detonation behavior in fuel-air mixtures.

6. Bibliography

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