Warsaw Univeristy of Technology

Faculty of Power and Aeronautical Engineering

Computer methods in combustion - Project

# Calculation of the detonation velocity of the methane-air mixture in a constant volume for variable initial parameters

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# Contents

# 1 Introduction

Detonation modeling begins from the Chapman-Jouguet (CJ) theory that appeared more than a hundred years ago and considered an ideal one-dimensional (1D) steady-state detonation wave. The theory does not provide any details about the reaction zone of the detonation wave, but it defines the ideal detonation velocity as a thermodynamic function which depends on the released energy and the equation of state, and does not depend of the kinetics of energy release. The next step in detonation modeling was made by Zeldovich, von Neuman, and Döring who considered a 1D steady-state detonation wave with a reaction zone of a finite thickness. According to the Zeldovich-Neumann-Döering (ZND) model, the energy release begins in a hot, shock-compressed material behind the shock front, and continues until the thermodynamic equilibrium is established. This equilibrium point at the end of the reaction zone corresponds to the CJ point in the Chapman-Jouguet theory. The detonation velocity in ZND model is still equal to CJ and independent of the kinetics of energy release which affects only the reaction-zone thickness. Both CJ and ZND models are based on exact solutions for 1D steady-state detonation waves, and therefore provide correct asymptotics for multidimensional theories of steady-state detonations. Both models are also used to check the accuracy of stable time-dependent numerical solutions. Calculated values of CJ velocity are very close to mean detonation velocities actually measured in experiments for large-diameter systems, providing that the equation of state of detonation products and the energy released in a detonation wave are well defined. As we can see, calculation of CJ velocity can be very helpful in defining more complex problem's solution.

# 2 Literature : scientific 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.

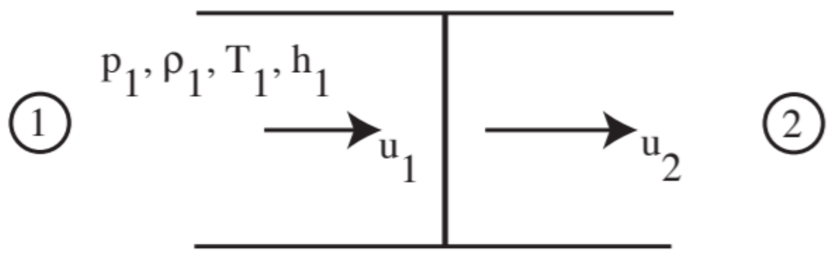


**Figure 1:** Coordinate system stationary to the wave

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:

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

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 $u_1, u_2, p_2, \rho_2$ 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:

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

Eliminating the velocity we get

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

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

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

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

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. 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 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 R-H curve. But are all physically realizable?

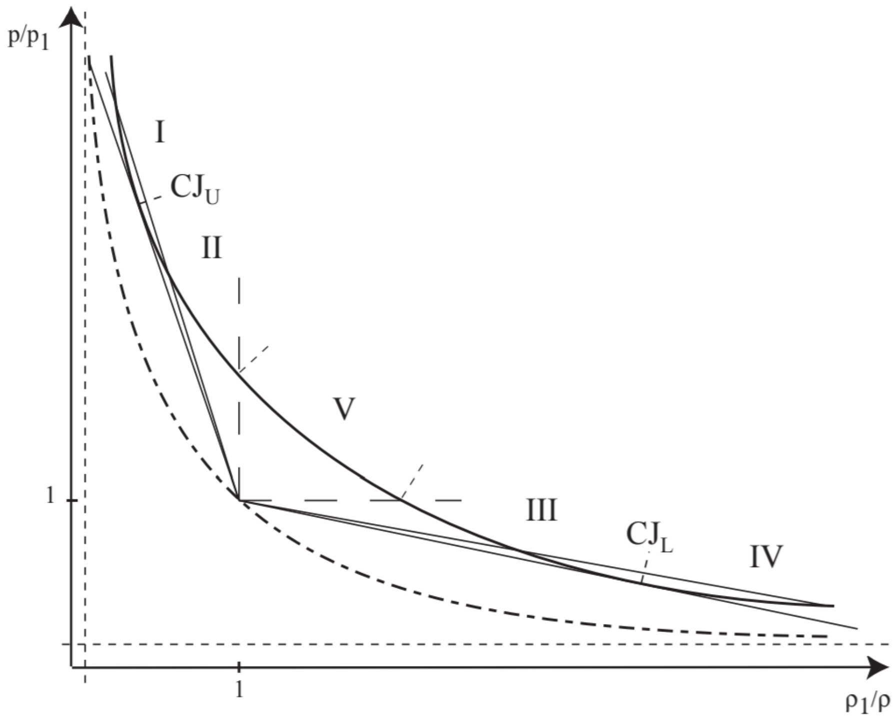


**Figure 2:** Rankine-Hugoniot curve and Rayleigh line. Straight lines are Rayleigh lines for different massfluxes. The dash-dot curve is the shock Hugoniot curve.

To discuss the matter we have divided the R-H curve into five segments, I−V .

**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 Chapman-Jouguet 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)

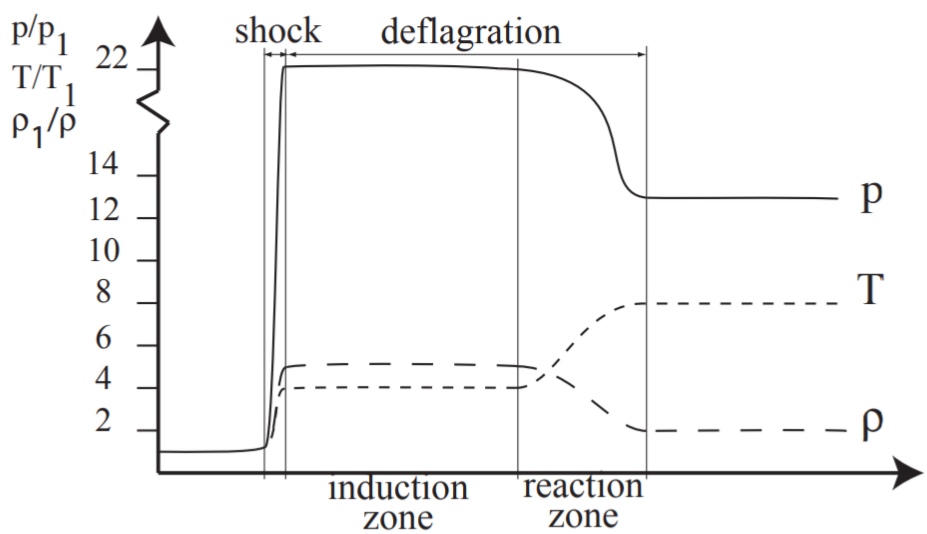


**Figure 3:** ZND wave

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 fig 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 $u_2^2 = a_2^2 = \kappa_2 R_2 T_2 = \kappa \frac{p_2}{\rho_2}$ we can finally obtain:

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

# 3 Modeling method description

To obtain the computation results of methane-air mixture detonation speed in constant volume the Shock & Detonation Toolbox software is used.

The Shock & Detonation Toolbox is a collection of numerical routines that enables the solution of standard problems for gas-phase explosions using realistic thermochemistry and detailed chemical kinetics. The SD Toolbox employs Dave Goodwin's Cantera software for the chemistry functionality and uses either MATLAB or Python (and related libraries) for scripting. The Cantera package provides conversion utilities from legacy formats in order to make use of existing databases of chemical kinetics and thermochemistry.

In this case I am using specifically the numerical routine for the computation of CJ detonation speed with Python interface.

To define simulation components' attributes such as thermodynamic and transport properties or the reaction rates GRI - 3.0 mechanism is used. The GRI - 3.0 is a chemical mechanism developed by the Gas Research Institute to model natural gas combustion, including full $NO_x$ chemistry. It is a compilation of 325 reactions involving 53 species. A particular feature of GRI - 3.0 is that it has been optimized as a whole towards targets related to methane and natural gas combustion.

Computation is held in nested loops with varying initial conditions of pressure, temperature and equivalence ratio. The initial conditions are within limits of 1 to 10 bar(a) for pressure, 300 to 1000 K for temperature and 0.5 to 1.5 for equivalence ratio.

# 4 Results

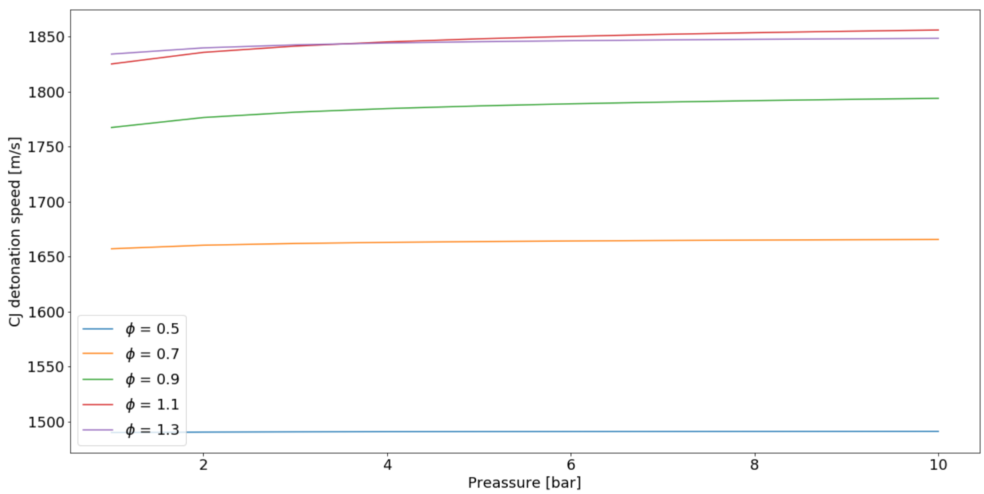


**Figure 4:** CJ detonation speed as a function of pressure, T1 = 300 K, $\phi$ = var

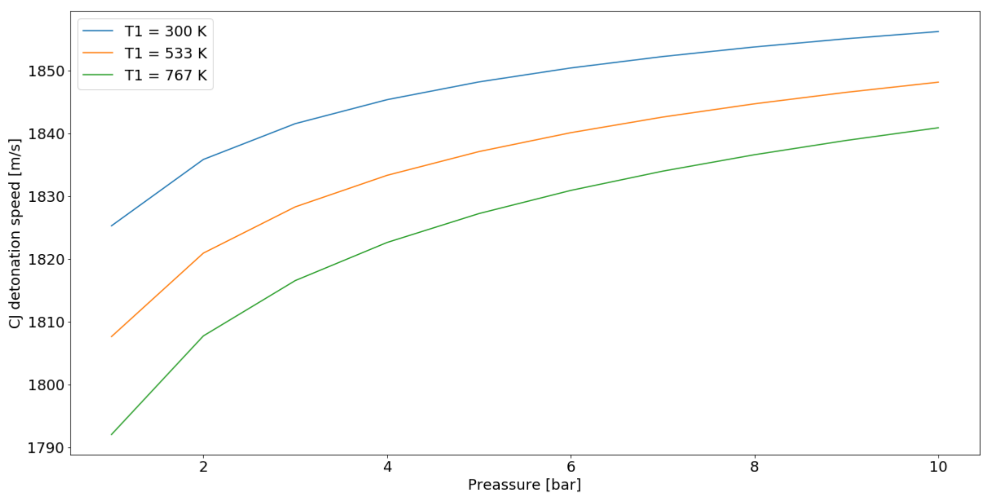


**Figure 5:** CJ detonation speed as a function of pressure, phi = 1.0, T1 = var

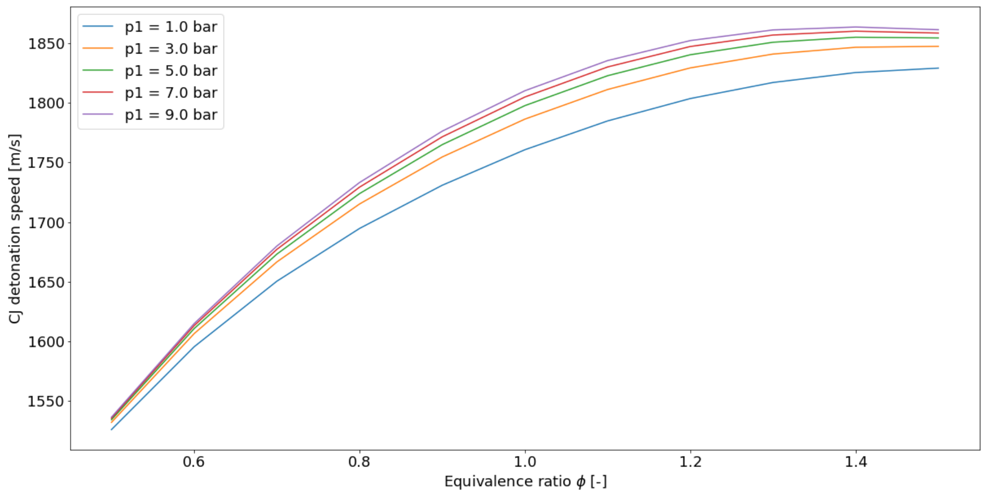


**Figure 6:** CJ detonation speed as a function of equivalence ratio, T1 = 883 K, p1 = var

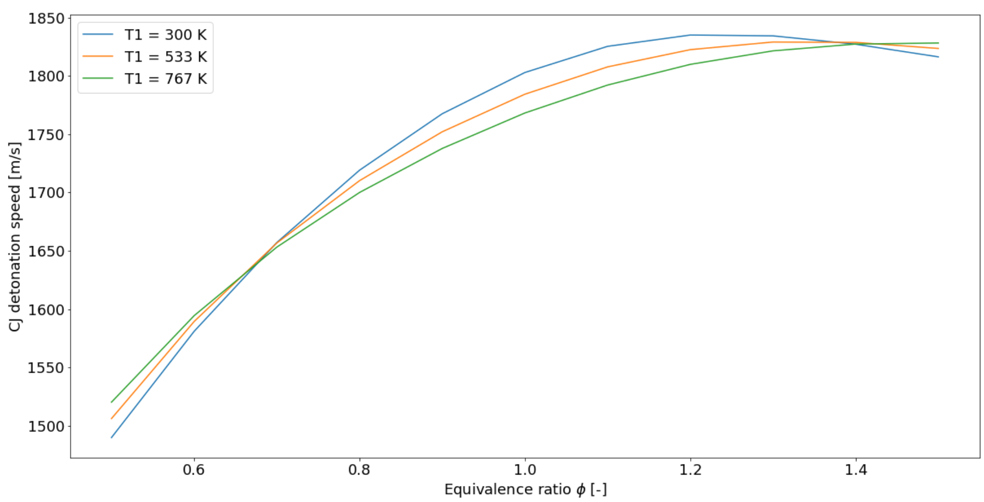


**Figure 7:** CJ detonation speed as a function of equivalence ratio, p1 = 1 bar, T1 = var

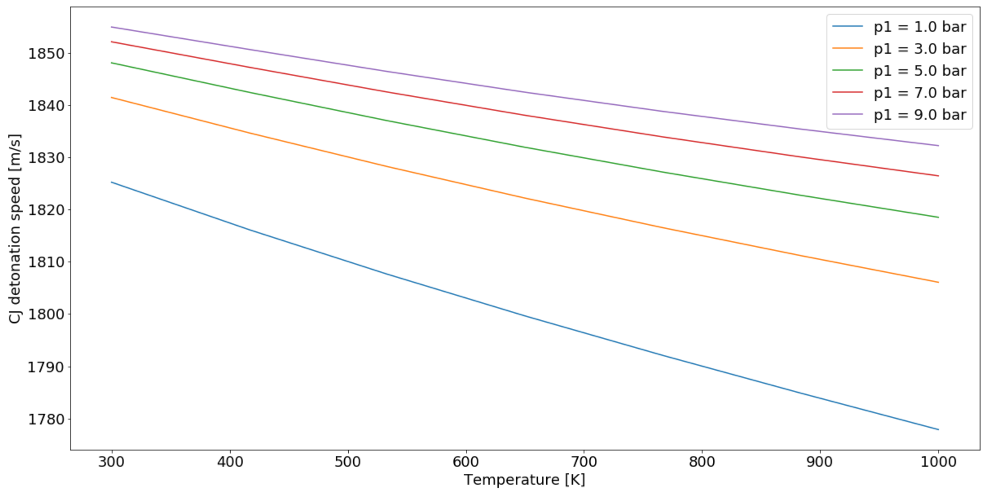


**Figure 8:** CJ detonation speed as a function of temperature, $\phi = 1.0$, p1 = var

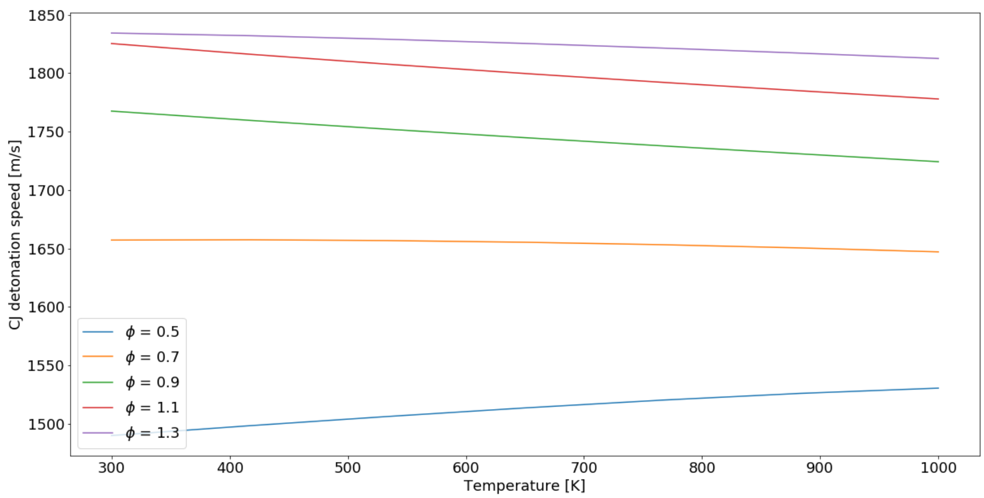


**Figure 9:** CJ detonation speed as a function of temperature, p1 = 1 bar, $\phi$ = var

# 5 Conclusion

From graphs 4 and 5 showing the effect of pressure, we can see that the increase in pressure causes a small increase in the value of the CJ detonation velocity (changes in the order of maximum 50 $\frac{m}{s}$ which is 2.8 % of changing value). Changes are larger when equivalence ratio is higher and when temperature is higher.

From graphs 6 and 7 showing the effect of equivalence ratio, we can see that increasing $\phi$ greatly increases CJ detonation speed, but the curve has a maximum from which the value begins to decrease. Maximum occurs around $\phi = 1.3$ for T1 = 300 K. As the temperature rises $\phi$ at which maximum occurs is higher. Also increasing initial pressure enhances the impact of equivalence ratio changes on detonation speed.

From graphs 8 and 9 showing the effect of temperature, we can see that increasing temperature causes a small decrease in the value of the CJ detonation velocity. Changes are larger when initial pressure is lower. Lowering equivalence ratio tends to change the trend of the curve to a growing one and enhance the level of value change. Increasing $\phi$ tends to change the trend of the curve to a decreasing one and also enhance the level of value change, but in other direction. For $\phi = 0.7$ the curve is almost flat.

# 6 Sources


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