Analysis of p-v plot in H2/O2 detonation

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1 Introduction

Pressure versus volume plot (p-v plot or diagram) is well knows graph to describe deflagration and detonation. Thermodynamic paths and planes of p-v plot had been well defined with equations. However, the ideal one-dimensional model known from Zeldovich, vol Neuman, and Döring (ZND model) theory differs from three-dimensional and two-dimensional p-v plot.
With just experiments it is a big challenge to look closely into some parameters. Nowadays, with numerical codes, it can be noted that thermodynamic paths differs from ZND model.
In this paper it will be explained how does p-v plot forms in two-dimensional case.

2 Method and theory basics

For non-reactive gases the first one to derive independently the relationship between the upstream and downstream states was Rankine [1] and Hugoniot [2].
When a perfect gas is assumed, it is possible to build the Hugoniot curve from p and v only:

$$y = \frac{\frac{\gamma_0 + 1}{\gamma_0 - 1} - x + 2q'}{\frac{\gamma_1 + 1}{\gamma_1 - 1} x - 1} \tag{1}$$

where $x = \frac{v_1}{v_0}$ $q' = \frac{q}{p_0 v_0}$. If q (or q') is equal zero then above equation becomes the Hugoniot curie for a non-reacting shock wave [3].
Typical p-v plot expresses four states of combustion (weak and strong deflagration, weak and strong detonation) that can be closed on one line one after another (Fig. 1).
In order to simulate deflagration, detonation, and its transition (deflagration-to-detonation transition - DDT) Navier-Stokes equations have been used. Stoichiometric mixture of oxygen and hydrogen fills the calculation domain, and a full chemical reaction model is provided with the Petersen and Hanson model with eight species (H2, O2, H, O, OH, HO2, H2O2, H2O) and eighteen reactions. The finite difference schemes used are a Harten-Yee, non-MUSCL modified-flux TVD method for the convective term, a point-implicit method for the production term, and a Strang-type time splitting method for the time integration term to keep a second order accuracy explicitly. The average values at the cell boundary are computed by the Roe-averaged method.

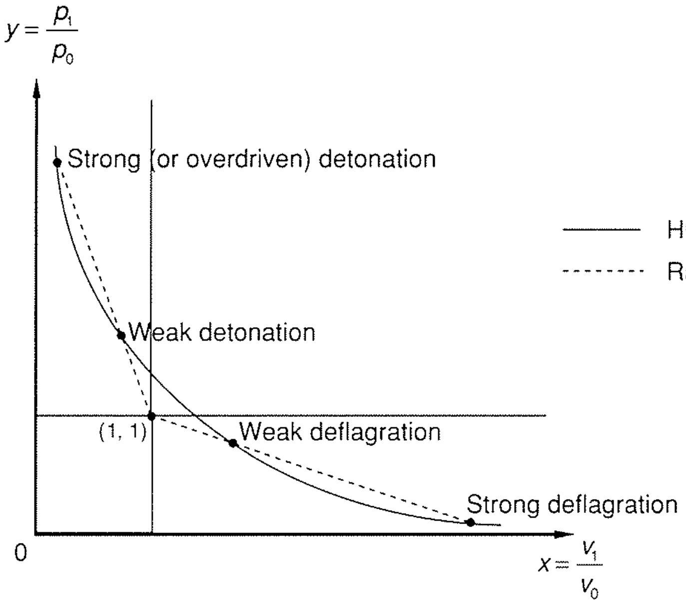


Figure 1. One-dimensional p-v plot presenting four states of combustion [3].

Calculation domain has rectangular shape of 2x45 mm, and is divided into three regions (Fig.2). Even though the small size of the model, detonation wave can be formed and propagate, which was proved by experiment before. This type of modeling lowers numerical cost a lot. Grid is build out of $7.5\text{x}10^6$ grid points. In x-direction size stays the same, however, for y-direction the smallest grid cells are at the walls and its size grows towards the axis. All walls are considered to be adiabatic besides right one, which is set an open end.

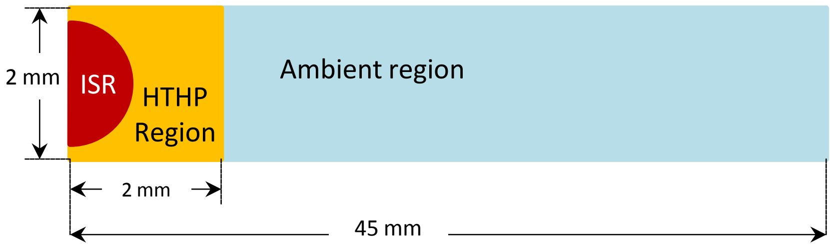


Figure 2. Calculation domain: IRS – Ignition Source Region; HTHP Region – High Temperature and High Pressure Region.

3 Results

At the beginning of propagation flame is laminar but as soon as it starts producing pressure and shock waves its shape changes to more wrinkled. A precursor shock is formed in front of the propagating flame and it propagates ahead of the flame not changing the distance. After some certain time autoignition happens in the boundary layer [4] and a new flame is developed. That new flame leads to DDT and detonation (Fig. 3).

In spite of very sharp images that are obtained by experiments as well as numerical simulations in reality shock wave is not a line but it has some certain thickness. That implements that shock wave's strength will be different at its head, tail, and inside (in the thickness). Measurement points for p-v plot are fixed to the shock. In our calculations we are able to distinguish four points that belong to the precursor shock structure. For that reason p-v plot, as well as Hugoniot curve are presented for four different locations in y-direction but on the same line of x-direction (axis). Figure 4 shows pressure and density ratio along the x-direction for the precursor shock at random moment of time at the axis for a small cutaway (between8053 and 8075 grid points). Point 1 represents a head of the precursor shock, point 4 a tail, and points 2 and 3 are located 'inside' the structure of the precursor shock. It means that for the results there are going to be four pressure records according to those four measurement points.

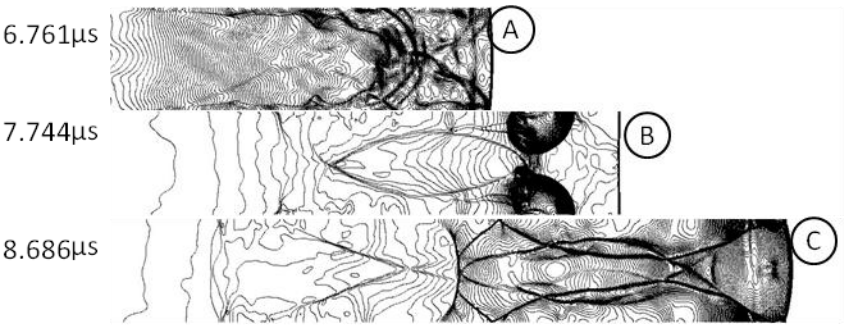


Figure 3. Pressure record for three different moments in time. A – state before autoignition and detonation; B – state after autoignition and before detonation; C – detonation.

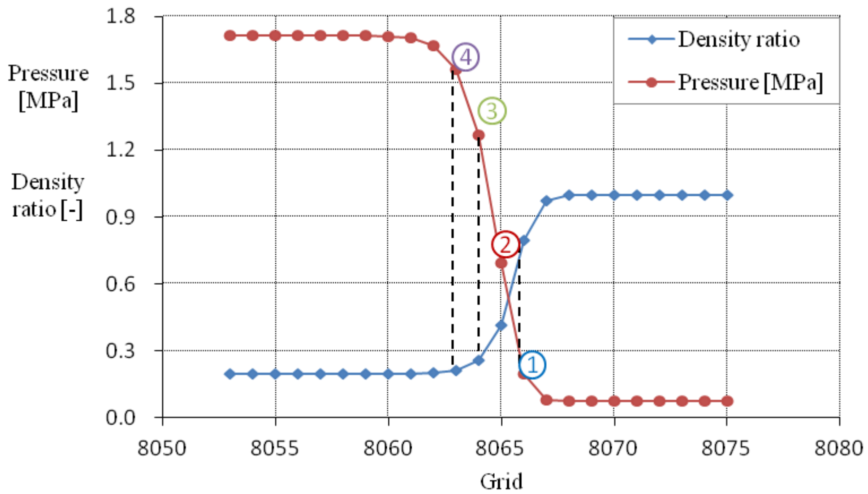
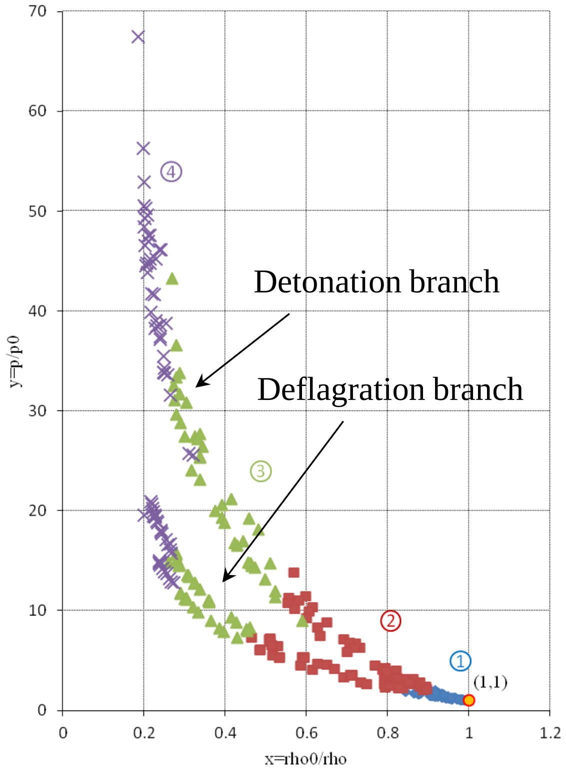


Figure 4. Pressure and density ratio obtained numerically through the precursor shock wave. 1 – head of the precursor shock wave; 2 and 3 – points 'inside' the precursor shock wave; 4 – tail of the precursor shock wave.

P-v diagram for four grid points belonging to the precursor shock structure can be seen in Fig. 5. The upstream state is marked with a circle (1,1). One can observe two Hugoniot curves built up from scattered points. Similar evaluation was delivered by Taylor et al. [4]. As the location 1 is at the head of the shock, results are closest to the upstream state. As the measurement locations changes towards the downstream state points are getting farther from the initial (1,1) state. The lower branch represents the deflagration state, while the upper one detonation. Many values for different points are obtained due to the changes of the precursor shock strength. It is possible to register such a phenomenon because the flame produces many shock waves, which propagate faster that the precursor shock, hit, and merge. Additionally the graph on the right side in Fig. 5 shows p-v plot with shock Hugoniot.



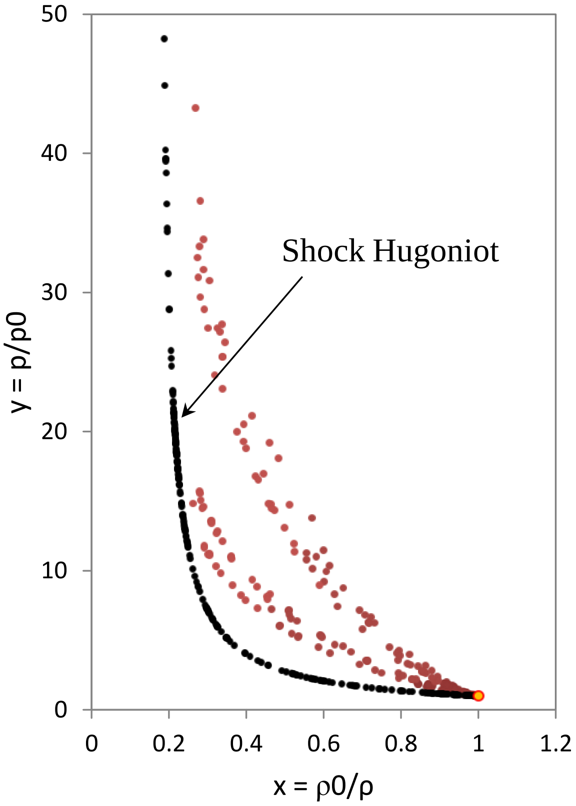


Figure 5. Left: p-v diagram for the pressure shock. 1 – head of the precursor shock wave; 2 and 3 – points 'inside' the precursor shock wave; 4 – tail of the precursor shock wave. Right: p-v diagram (the same as the left figure) with shock Hugoniot.

Formation of deflagration and detonation branches for the p-v diagram are shown in Fig. 6 and 7 respectively. Surprisingly points do not appear in a sequence one after another but in some sort of chaotic order. They can still be closed into some line-like shape; however, the order of appearance is random and dictated by the strength of the precursor shock. When the detonation wave takes over the precursor shock, the upper branch is formed exactly in the same chaotic way as the deflagration part.

4 Conclusions

This work is aimed to show that theoretical p-v plot differs from the real one. It cannot be closed into one line that passes through the initial state condition's point. Instead two branches are formed. Lower one represents deflagration state, and the upper one detonation. The strength of the shock is changing and for that reason p-v plot formation process is not linear.

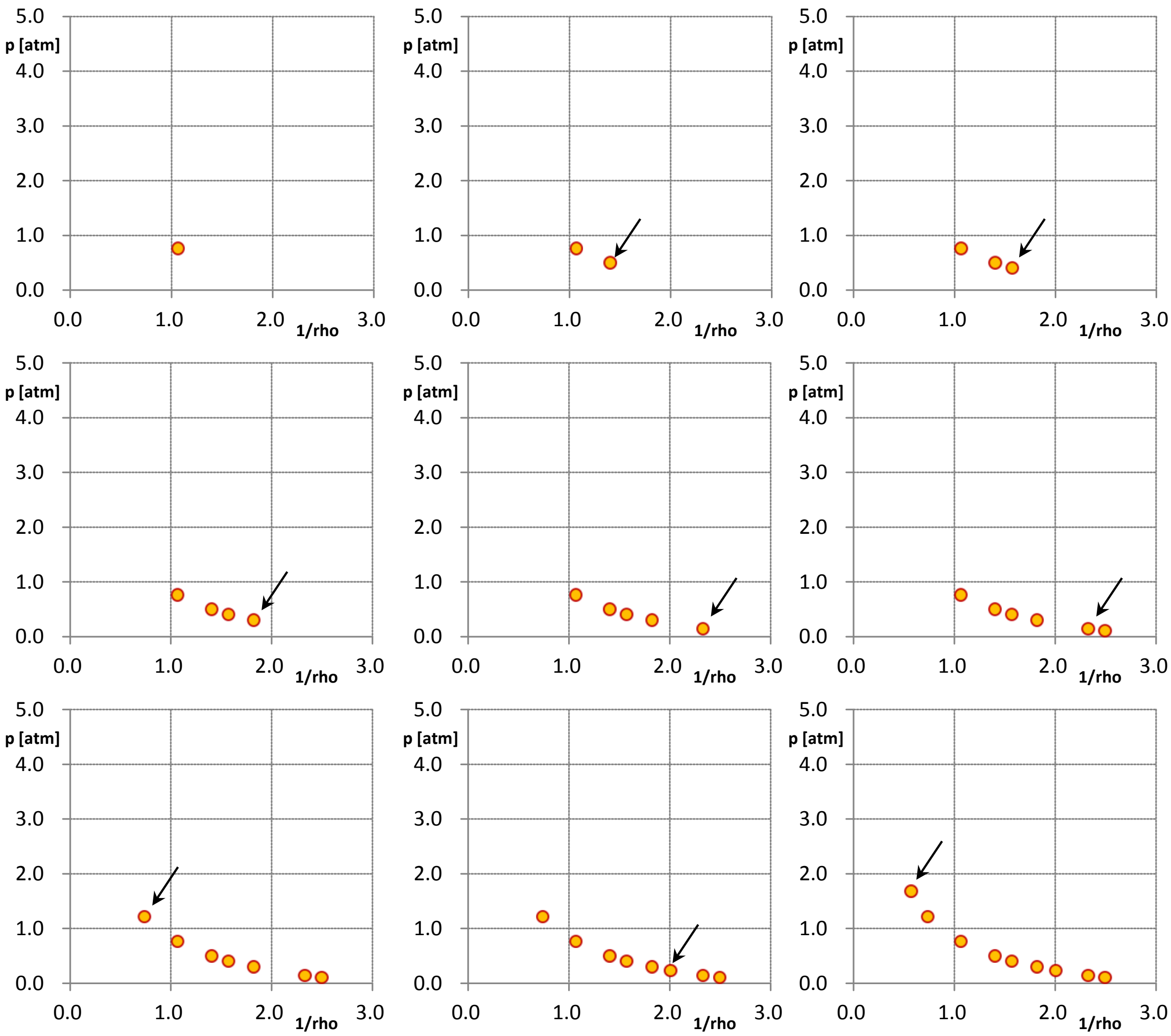


Figure 6. Formation of the deflagration branch of the p-v plot.

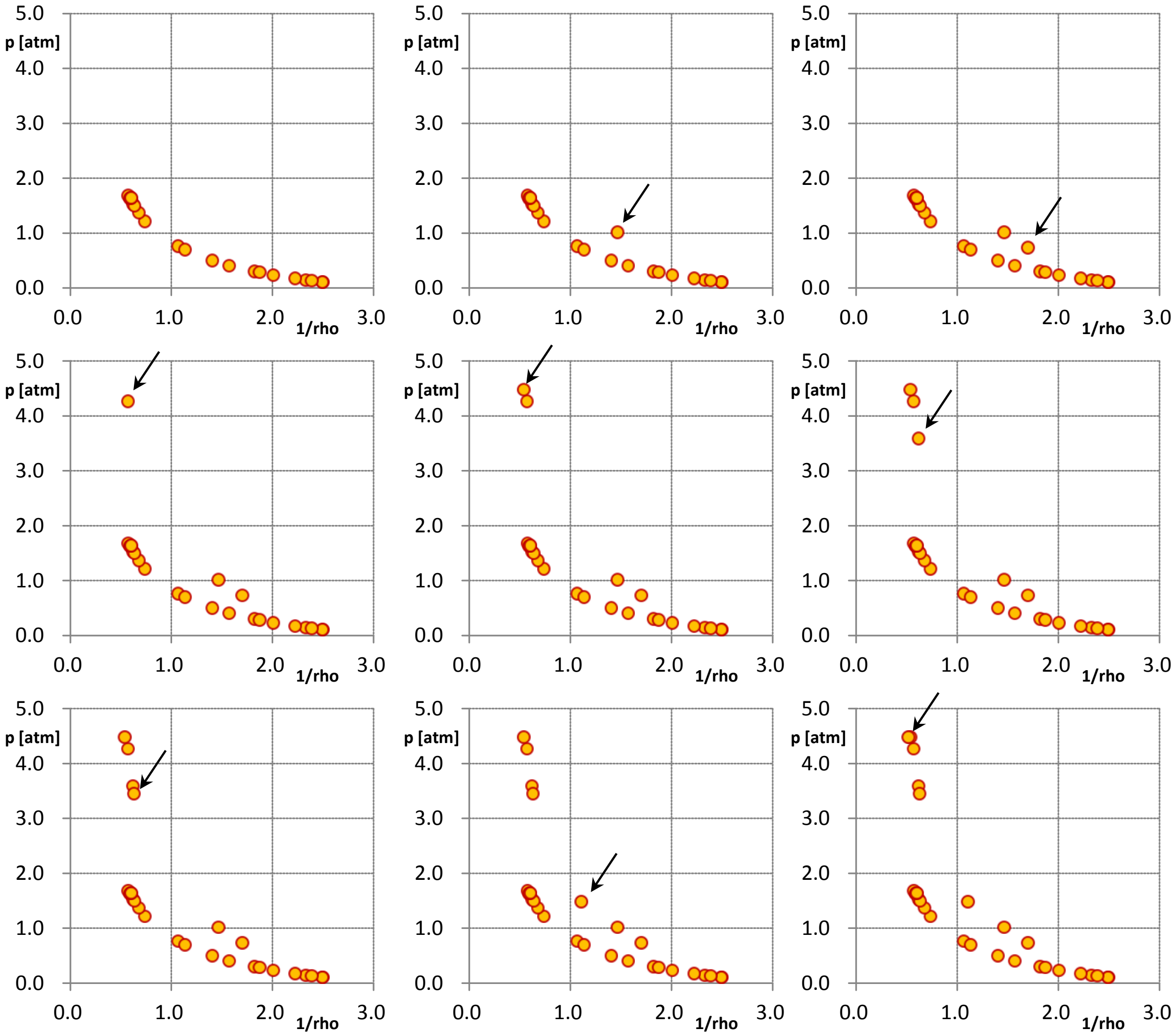


Figure 7. Formation of the detonation branch of the p-v plot.

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