A NUMERICAL STUDY OF PLANAR DETONATIONS

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Abstract. A one dimensional numerical study on the build-up and propagation of planar detonation waves in H_2 and Air combustibles mixtures is presented. To describe the motion of a traveling detonation the unsteady Euler equations coupled with source terms to account for a finite rate chemical activity, are used. The algorithm for computing the numerical hyperbolic fluxes is based on the Harten-Yee TVD scheme. Since the source terms lead to stiff differential equations, an implicit treatment of these terms is implemented. The computer solver works with 13 chemical species and 33 different one step reactions of a $H_2 - O_2 - N_2$ combustion mechanism. The detonation process is initiated via the energy provided by an igniter made of hot and high pressure helium which acts as a driver of a shock tube driving through a combustible mixture a blast (or strong shock), accompanied by exothermic chemical changes. It is shown that for each equivalence ratio of the combustible mixture, the detonation can only be triggered if the igniter energy deposition is equal or exceeds a computed minimum value. When the igniter energy deposition is less than this minimum, the combustion zone decouples from the blast wave. This blast, as it travels downstream becomes weaker and no longer induces chemical reactions across it, however, a chemical activity still remains being now started by a reaction front located at some distance behind the leading wave. Finally, a particular way of generating an overdriven detonations is considered.

Key words: unsteady flow, chemically reacting flows, TVD numerical scheme, chemical kinetics, ignition, propagation, Chapman-Jouguet detonations, overdriven detonations

1 INTRODUCTION

It is well known that any explosive mixture, can in general, go through two extremes modes of combustion. One extreme is the slow laminar deflagration mode; here the flame propagates at typical velocities of the order 1 ms^{-1} relative to the unburned gases and the overpressure is small. The other extreme is the detonation mode, in which the detonation wave propagates at velocities of the order of 2000 ms^{-1} and with an overpressure rise across the wave of almost 20 times the initial value. The propagation of laminar deflagrations is governed by the molecular diffusion of heat and mass fron the reaction zone to the unburned mixture. On the other hand, the propagation of detonations depends on the adiabatic shock compression of the unburned mixture to increase its temperature to bring autoignition. The strong exponential temperature dependence of chemical reactions rates, makes possible the rapid combustion in the detonation mode. In between the two extremes of laminar deflagration and detonation, theres is an almost continuous spectrum of burning rates, however in this work, only detonations in homogeneous gaseous mixtures of H_2 and Air are considered.

The classical Chapman-Jouguet theory, seeks the unique solution of the one-dimensional conservation equations across the detonation front in which the flow behind the wave is sonic. It involves only an equilibrium thermodynamic calculation for the detonation states (i.e. the detonation velocity, pressure, temperature, and density ratios across the wave, and the equilibrium composition of the products gases). These detonation states calculated using the classical approach agree well with experimental observations. However, parameters like the iniciation energy, detonability limits, the thickness of the reaction zone and the critical tube diameter, are requiring a knowledge of the structure of the wave itself, and hence the chemical reaction rates. Following Lee (1984), these parameters are refered as the *dynamics detonation parameters* to distinguish from the equilibrium *static* detonation states obtained from the Chapman-Jouguet theory.

A century after the formulation of the successful Chapman-Jouguet theory, the estimation of *dynamics detonation* parameters continues being mostly, based on experimental data, see Kaneshige and Shepherd (1997). In the 1960s, experiments revealed that gas-phase confined detonations are most often characterized by unsteady, three-dimensional cellular estructures, which can only in an averaged sense be predicted by one-dimensional steady theories. Since then, numerical modeling has steadily advanced to predicting the flow field behind shock induced reactions (Sharpe and Quirk (2008)), nevertheless and to the degree of our knowledge, no theory has yet described how the structure is formed and sustained behind unconfined waves. In this context, a study on starting and propagating planar unconfined detonations waves, based on solving unsteady flow equations coupled with finite rate chemical processes, has been carried out.

To start a detonation as a *planar wave* and to keep it always like that, a *planar igniter* shall also be used. Such igniter has been conceived as a region adyacent to the closed end of the detonating system, filled with high temperature and high pressure helium (He). Then, the igniter can function as the driver of a shock tube (Tamagno et al. (2003)), and use its energy to drive through a combustible medium a front blast (or strong shock) accompanied by exothermic chemical changes. This setup show consistency with the main objectives of this work: 1) to determine the energy that must be used to initiate a self sustained Chapman-Jouguet *planar detonation*, and in case of an overdriven start it shall decay to a Chapman-Jouguet state; 2) to verify that when the igniter energy is lower than the critical value for direct initiation, the combustion zone decouples from the blast front; 3) to generate a sustainable overdriven detonation.

This numerical study of planar detonations in $H_2 - Air$ combustible mixtures, is accomplished by solving time dependent one-dimensional Euler equations with source terms. The source terms are needed to account for the finite rate chemical activity between the constituent gases. The computer code allows the incorporation of 13 chemical reacting species (N_2, O_2, H_2, NO, OH, NO_2, HNO, HO_2, H_2O, H_2O_2, N, O, H). The igniter helium (He) is added as an inert species. The finite-rate chemistry mechanism describing the detailed chemical kinetics of the hydrogen oxidation in air assembled by Jachimowski (1988), is adopted. The approach taken to numerically solve the non-linear systems of hyperbolic conservation laws is based on a finite-volume form of a second orden Harten and Yee TVD scheme Yee (1989). Regarding the source terms, it shall be noted that chemically active flows contain a range of widely varying time scales which leads to *stiff* differential equations. Usually, the problem of stiffness may be resolved by resorting to implicit methods. However, for chemically active flow models stiffness may not be resolved by simply using implicit techniques. If the mesh is not sufficiently fine in both space and time, spurious unphysical solutions may be computed (Toro (2009)). The implicit algorithm here employed is recognized as a *point implicit approach* since it treats only the source terms implicitly (Wilson (1992)). More details about the system of one-dimensional governing equations, the chemical source terms and its implicit treatement, are given in Tamagno et al. (2010).

2 RESULTS OF THE NUMERICAL STUDY

Experimentally, it is found that for a given mixture at given initial conditions, a definite quantity of energy must be used to initiate a detonation "instantaneously". By "instantaneously" is meant that the initial blast (or strong shock wave) generated by the igniter after the rapid deposition of its energy, decays to a Chapman-Jouguet detonation (Lee (1984)). If the igniter energy is less than a certain value, the combustion zone progressively decouples from the front blast as it decays. Applying the numerical approach previously described to a planar starting and propagating blast both aspects, the tendency of the initial blast wave generated by the igniter to becoming a Chapman-Jouguet phenomena or the decoupling of the reaction zone from the blast, are intended to be simulated. In addition, a way of starting and sustaining an overdriven detonation is presented. Note that for an inviscid and adiabatic truly planar flow, the geometry which contains it becomes irrelevant.

2.1 The start and the propagation of a planar detonation wave

Let us consider first, a stoichiometric mixture of $H_2 + Air$. Fig. (1) shows in coordinates $time$ vs. $distance$ the blast (or shock) starting by the igniter and then propagating downstream the tube as a detonation wave (DW). Here the planar igniter or ignition source is materialized by a small region of length $2.5\,mm$ located at the closed end of the detonating system, filled with hot and high pressure helium. The temperature of the hot helium was fixed at $3900\,K$ and the pressure is varied from $1.0\,e+06$ up to $4.0\,e+06\,(Pa)$ depending on the equivalence ratio (ER) of the $H_2 + Air$ combustible medium used. The number of cells used in $0.40\,m$ of field length was 1600 and the time steps 520000. These large number of cells and the high number of time steps needed to obtain what are believed physical meaningful answers ($CFL = 0.004$), are consistent with Toro (2009) statement that in chemical reacting flows not always the problem of stiffness may be resolved by simply applying implicit techniques.

In Figs. (2) and (3) are presented pressure and temperature distributions along the tube after 0.21 milliseconds of flow time. The pressure as expected, behaves like a Taylor expansion

wave, showing a peak at the location of the DW and a minimum value as it approaches the closed end of the detonating system ($X = 0.0$). The temperature behavior, describes the jump across the DW due to heat release by exothermic chemical reactions, as well as the interface that separates combustion products from igniter gases. The corresponding O_2 depletion and the H_2O formation, are shown in Figs.(4).

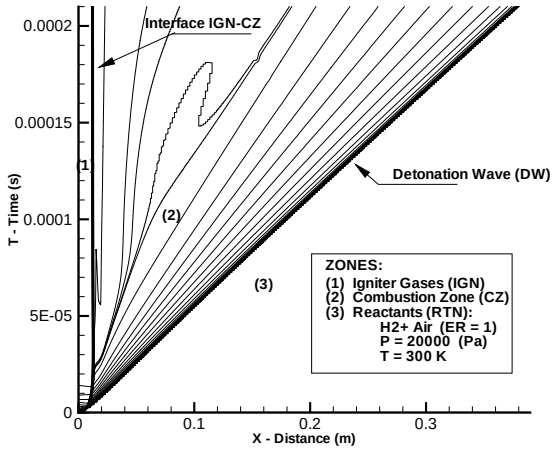

Figure 1: Computed X-T diagram of the logarithm of constant density contours - Ign. Pres.: 1.5e+06(Pa).

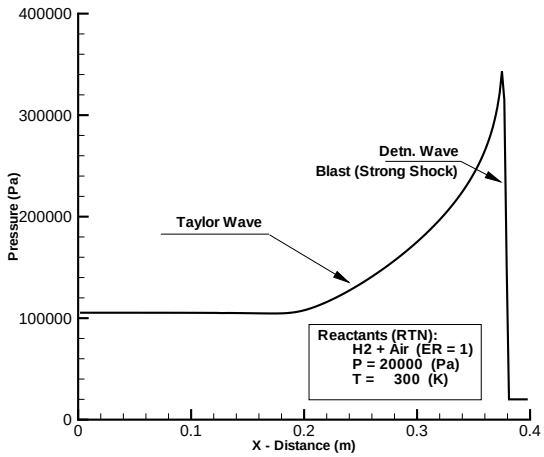

Figure 2: Computed, pressure as function of distance at flow time=2.1 e-04(s) - Ign. Press: 1.5e+06(Pa).

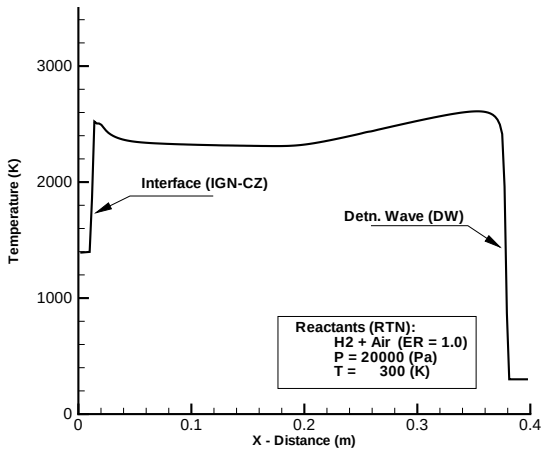

Figure 3: Computed, temperature as function of distance at flow time=2.1 e-04(s) - Ign. Press: 1.5e+06(Pa).

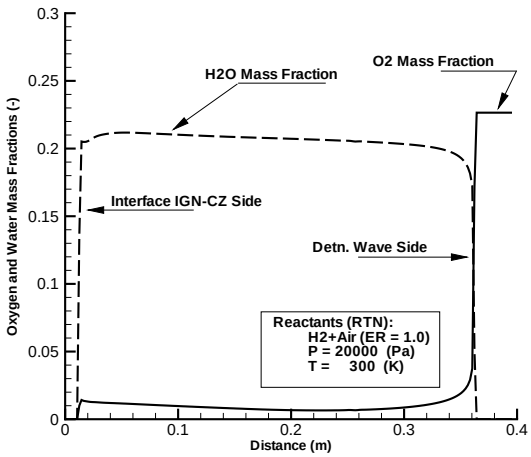

Figure 4: Computed, oxygen and water mass fractions as function of distance at flow time=2.1 e-04(s) - Ign. Press: 1.5e+06(Pa).

The results up to know presented, are applicable to a $H_2 + Air$ stoichiometric mixture. Also, identical calculations with this combustible mixture at $ER = 0.5$ and $ER = 2.0$, are made. Of particular interest is the comparison between detonation velocities computed using Chapman-Jouguet equilibrium calculations (Gordon and McBride (1971), Gordon and McBride (2005),

Scarpin (2006)), and using finite rate chemistry. It can be concluded from Fig.(5), that the equilibrium and finite rate calculated velocities of DWs agree satisfactorily.

2.2 The decoupling of the reaction zone from the blast

Calculations for the stoichiometric H_2+Air mixture have shown that to produce a Chapman-Jouguet detonation wave, the igniter energy deposition shall not be less than $3000\,Joules/m^2$. If this energy deposition does not reach the minimum value, then, the combustion zone should decouple from the initial blast. To verify this statement, the igniter energy is reduced to $2800\,Joules/m^2$ and the computer program is run with this value. Fig.(6) shows, in coordinates $time\ vs.\ distance$, the results obtained.

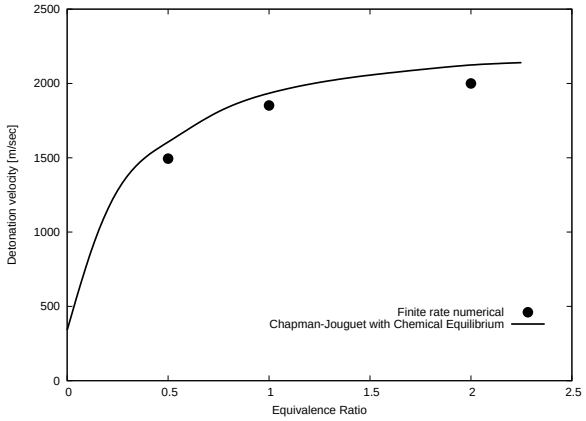

Figure 5: Comparison between detonation velocities computed using Chapman-Jouguet equilibrium and finite rates

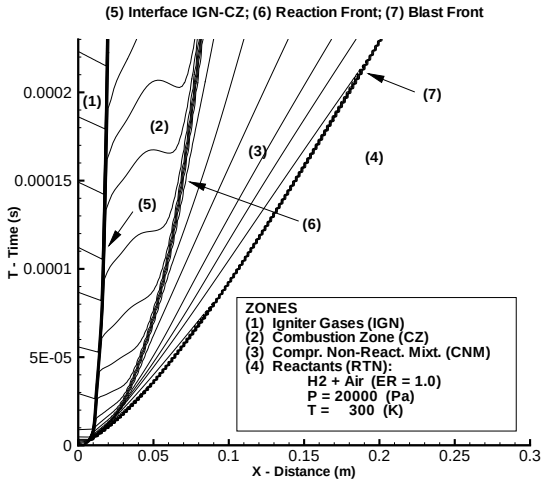

Figure 6: Computed, X-T diagram showing the combustion zone decoupled from leading blast - Ign. Press.: 1.13e+06(Pa).

After the blast (7), a non reacting compressed region (3) develops. Although the pressure in this region (see Fig.(7)), also peaks immediately after the shock and progressively diminish toward the closed end, it shall be noted that the ratios $pressure\,/\,reactants\ pressure$ at its peak and elsewhere in region (3), are smaller than the corresponding ratios obtained with a detonating stoichiometric $H_2\ +\ Air$ mixture (by a factor of 5.3 at the peak and of 3.4 at the closed and). A computed temperature distribution along the tube is plotted in Fig.(8). A sort of a *reaction front* (6), separating the combustion zone (2) from the zone (3), can be detected. In addition, the interface igniter-combustion zone is positioned. Fig.(9) shows computed mass fractions of oxigen and water vapor.

2.3 Generation of an overdriven detonation

To generate a sustainable overdriven detonation traveling at a greater speed than the corresponding Chapman-Jouguet detonation, the hot and high pressure helium igniter is now assumed to be unlimited. The temperature and pressure of the igniter gas are $3900(K)$ and $1.0\,e+06\,(Pa)$, respectively. This igniter will drive an hypothetical shock tube whose driven gas is a combustible H_2+Air mixture of $ER=1.0$, has a pressure of $20000(Pa)$ and a temperature of $300\,(K)$. Since it is assumed that the shock tube process is non diffusive, the interface

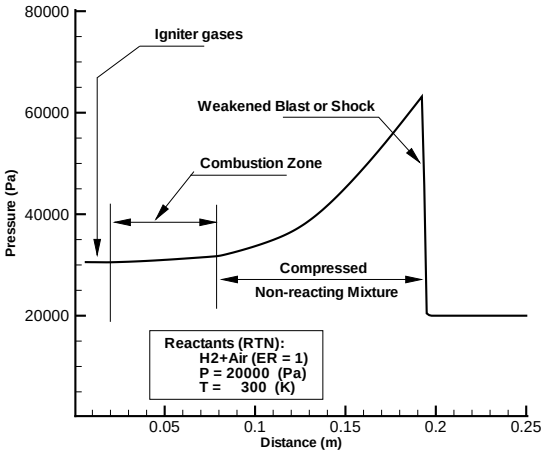

Figure 7: Computed, pressure as function of distance at flow time=2.2 e-04(s) - Combustion zone decoupled from leading blast.

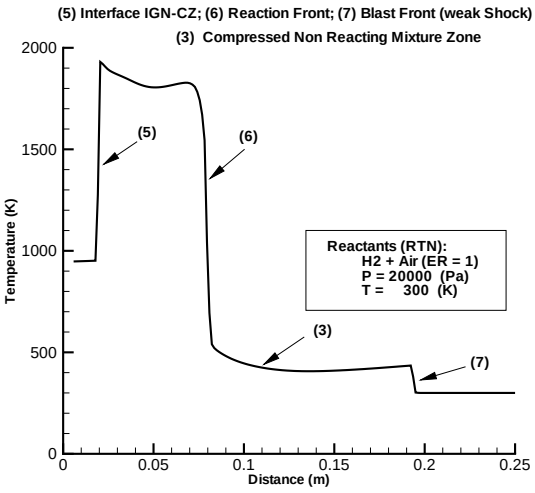

Figure 8: Computed, temperature as function of distance at flow time=2.2 e-04(s) - Combustion zone decoupled from leading blast.

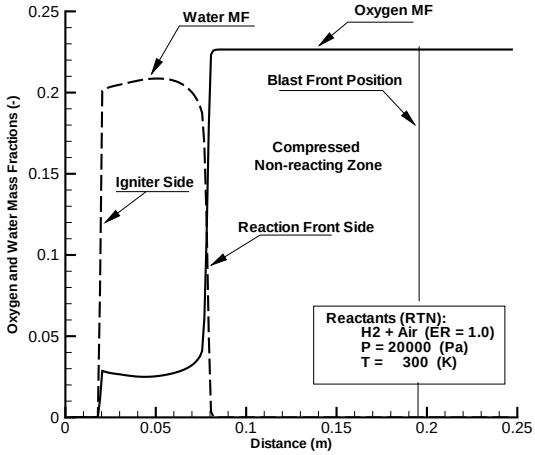

Figure 9: Computed, oxygen and water mass fractions as function of distance at flow time=2.2 e-04(s) - Combustion zone decoupled from leading blast.

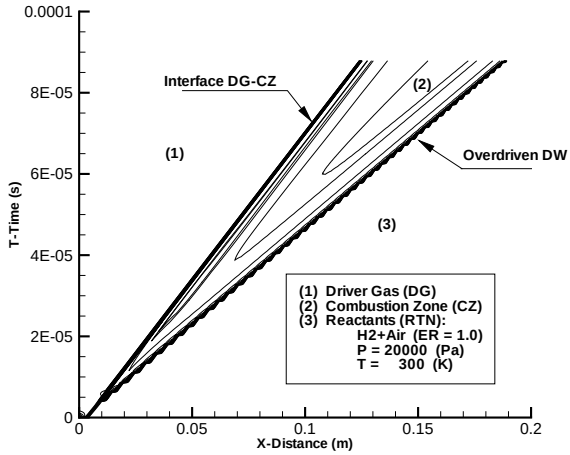

Figure 10: Computed, X-T diagram of the logarithm of constant density contours - Overdriven detonation.

between the igniter and driven gases can be considered as a “piston” whose mass equals that of driven cells (Acosta and Tamagno (2004)). This piston, shock compress adiabatically the combustible mixture to elevate its temperature to bring autoignition. Fig.(10) shows, in *coordinates time vs. distance* the results obtained. Figures (11) and (12), built on data taken at a flow time of $8.0\,e-05\,(s)$ depict, respectively, the velocity and pressure behavior which show consistency with the interface-piston concept of driving through the combustible mixture a strong shock. The exothermic chemical change can be inferred by the depletion of oxygen and the water vapor formation (Fig. (13)).

The overdriven detonation here described, propagates at a velocity of $2118\,m/s$ and the Chapman-Jouguet detonation previously described in subsection [2.1], makes it at $1872\,m/s$ (see Fig.(5)). The relative Mach number behind the detonation no longer approaches the sonic

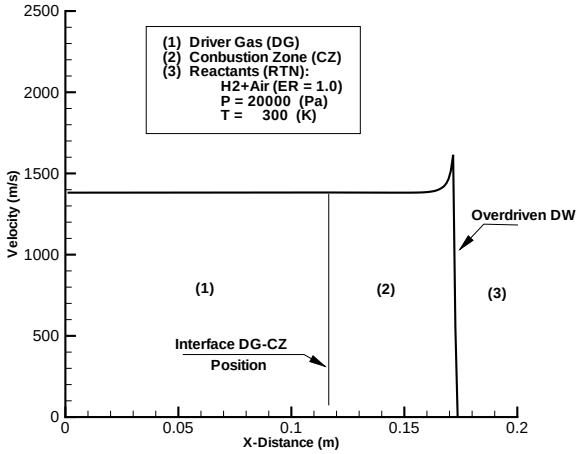

Figure 11: Computed, velocity as function of distance at flow time=8.0e+05 (s) - Overdriven detonation.

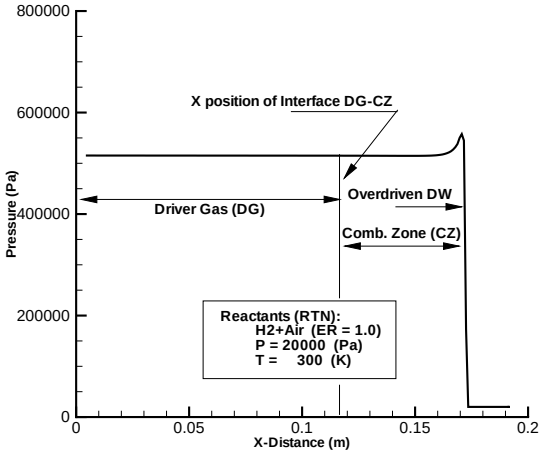

Figure 12: Computed, pressure as function of distance at flow time=8.0e+5 (s) - Overdriven detonation.

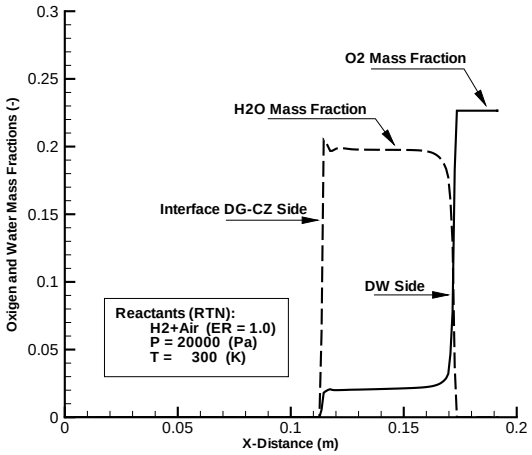

Figure 13: Computed, oxigen and water vapor mass fractions as function of distance at flow time=8.0 e-05(s) - Overdriven detonation.

value as it does in the Chapman-Jouguet case, instead, it remains definitively subsonic.

3 CONCLUSION

A numerical study concerning the start and the propagation of planar detonation waves, has been carried out. The numerical formulation solves the appropriate, unsteady Euler equations coupled with source terms to account for finite rates chemistry. 13 species and 33 one step chemical reactions of a $H_2 - O_2 - N_2$ combustion mechanism are considered. To totally preserve the concept of *planar* flow including the ignition source, this source or igniter is conceived as a driver of a shock tube that will adiabatically compress unburned combustible mixtures of $H_2 + Air$ raising its temperature beyond autoignition. Once started, the detonation becomes

self sustained and can travel large distances, unless limited by unaware causes to the flow, e. g. computing time. With the exception of the overdriven case, in all others, the interface igniter-combustion zone always has remained confined within a small region (of few centimeters downstream of its initial position).

The accomplished main objectives are:

1. Quantification of the minimum igniter energy deposition required to initiate, either in lean $(ER = 0.5)$, stoichiometric $(ER = 1.0)$ or reach $(ER = 2.0)$ combustible $H_2 + Air$ mixtures, a self sustained planar Chapman-Jouguet detonation. When the overdriven start of a detonation is not supported, it is proved that it always decay to a Chapman-Jouguet state. When this happen, the igniter pressure has dropped from its initial maximum value to the minimum one that gives the Taylor wave corresponding to this state. Furthermore, this pressure equalization limits the expansion of the gaseous igniter and fixes the position of the interface igniter-combustion zone.

2. Verification, that when the igniter energy is smaller than the minimum amount needed for direct initiation of the detonation, the combustion zone decouples from the blast front. A non reacting compressed region develops immediately behind a weakened blast and thereafter, a combustion region is positioned. Then, a sort of reaction front and its associated temperature jump, can be detected at the interface between these two regions.

3. Production of a sustainable overdriven detonation wave after adapting the planar igniter used in [1.] and [2.] to support it, and considering the interface as a piston that shock compress the combustible mixture to induce exothermic chemical changes.

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