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NUMERICAL SIMULATION OF DETONATION WAVES

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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 treatement 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 (the He is considered an inert species). The helium remains confined within a small region (no greater than a few centimeters), while the detonation continues until much bigger distances determined only by computing times. 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 (or shock) wave. This shock, 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 from the leading wave.

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 elevate 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 only detonations in homogeneous gaseous mixtures of H_2 and Air are considered in this work.

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 more complex model was proposed in the early 1940s by B. Zel'dovich, W. Döring and J. von Neumann. This model (now known as ZDN theory), permits the computation of the dynamics parameters when a model for the physical process involved is given. However, results provided by the ZDN theory are in disagreement with experiments. A century after the formulation of the successful Chapman-Jouguet theory, the estimation of *dynamics detonation* parameters continues being mostly, based on experimental data (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. 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 is conceived as a small adjacent region to the closed left side of the detonating system, filled with high temperature and high pressure helium. It is expected then, that the igniter will behave as the driver of a shock tube (Tamagno et al., 2003)), driving through a combustible medium a front blast accompanied by exothermic heat release. Consequently, the main objectives of this work are: 1) to determine the quantity of 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.

Numerical simulations of planar detonations in $H_2 - Air$ combustible mixtures, are 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 $(N_2, O_2, H_2.NO, OH, NO_2, HNO, HO_2, H_2O, H_2O_2, N, O, H)$. Helium (He) is added as an inert species with a prescribed third body efficiency. Even though finite-rate chemistry mechanism describing the detailed chemical kinetics of the hydrogen oxidation in air have been developed by a number of authors, in this study, the chemical mechanism 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, 1992a).

2 GOVERNING EQUATIONS

The resulting system of one-dimensional governing equations may be written in the following form

$$\mathbf{U}_t + [\mathbf{F}(\mathbf{U})]_x = \mathbf{S}(\mathbf{U}) \tag{1}$$

where $\mathbf{U}$ is the vector of unknows, $\mathbf{F}(\mathbf{U})$ is the vector of fluxes and $\mathbf{S}(\mathbf{U})$ is the vector of sources which is an algebraic function of $\mathbf{U}$ or other physical parameter of the problem at hand. These vectors are defined as follows

$$\mathbf{U} = \begin{pmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_{14} \\ \rho u \\ E_v \\ E \end{pmatrix} \qquad \mathbf{F}(\mathbf{U}) = \begin{pmatrix} \rho_1 u \\ \rho_2 u \\ \vdots \\ \rho_{14} u \\ \rho u^2 + p \\ u E_v \\ u\,(E+p) \end{pmatrix} \qquad \mathbf{S}(\mathbf{U}) = \begin{pmatrix} \dot{w}_1 \\ \dot{w}_2 \\ \vdots \\ \dot{w}_{14} \\ 0 \\ \dot{w}_v \\ 0 \end{pmatrix} \tag{2}$$

The density of each one the species is indicating by ρ_i and the overall density with $\rho = \sum_i \rho_i$. The other terms are the pressure p, the velocity component u, the vibration energy E_v and the total energy per unit volume E. The production or destruction of species i through chemical reactions is represented by the source terms $\dot{w}_i$, and the source vibration energy by $\dot{w}_v$. The relationship between pressure and temperature is given by the equation of state for a mixture of thermically perfect gases. That is

$$p = \sum_{i=1}^{14} \frac{\rho_i}{M_i} \mathrm{R}\,T \tag{3}$$

where R is the universal gas constant, M_i the molecular weight of species i and T the mean temperature of the mixture.

The total energy can be written

$$E = \sum_{i=1}^{14} (\rho\, C_v)_i\, T + \sum_{i=1}^{14} \left(\rho\, h^0\right)_j + E_v + E_{el} + 0.5\,\rho\, u^2 \tag{4}$$

In eq. (4), the first term is the sum of the translational and rotational energies per unit volume for each species, being $(C_v)_i$ its rotational and translational specific heat. The second term expresses the chemical energy per unit volume and the last term the kinetic energy, also per unit volume. E_{el} is the sum of the energy in the excited electronic modes and E_v contain the sum of the vibration energies for all species. These vibration energies are computed following Wilson (1992b).

2.1 On the chemical source terms

In general chemical reactions can proceed in both the forward direction (reactants forming products, rate constant k_f) and in the reverse direction (reaction products reforming the reactants, rate constant k_b). For each elementary reactions involving N species, the set of opposing chemical reactions can be written in the form, see Penner (1957); Williams (1965),

$$\sum_{j=1}^{N} \nu_j^{'} \mathrm{C}_j \xrightarrow{k_f} \sum_{j=1}^{N} \nu_j^{''} \mathrm{C}_j \tag{5}$$

$$\sum_{j=1}^{N} \nu_j^{'} \mathrm{C}_j \xleftarrow{k_b} \sum_{j=1}^{N} \nu_j^{''} \mathrm{C}_j \tag{6}$$

The $\nu_j^{'}$ are the stoichiometric coefficients for the reactants, and the $\nu_j^{''}$ represent corresponding coefficients for the reaction products. C_j is a chemical symbol to identify species j (in this case it is assumed that it represents *number of moles per unit volume*).

According to the law of *mass action*, the rate of production of a chemical species is *proportional* to the products of the concentrations of the reacting species, each cooncentration being raised to a power equal to the corresponding stoichiometric coefficients. Thus, for the *forward* chemical process described in eq.(5)

$$\text{reaction rate} = k_f \prod_{j=1}^{N} (\mathrm{C}_j)^{\nu_j^{'}} \tag{7}$$

The proportionality constant k_f is called the specific reaction-rate *constant* or *coefficient*. For a given chemical reaction the reaction rate constant k_f es independent of the concentrations, and depends only on the temperature. In general k_f is given by an expresion of the form (Williams, 1965).

$$k_f = B\, T^{\alpha}\, exp(E_A/\mathrm{R}T) \tag{8}$$

where the *frequency factor* B, the quantity α, and the *activation energy* E_A are parameters determined by the nature of the elementary reaction considered. However, throughout this study k_f will be regarded as an empirically determined coefficient which depends only on the temperature.

The only observable results of a chemical reaction are net rates of change for the chemical components. From eqs. (5) and (7) the net rate of production of C_i due to the chemical reaction proceeding in forward direction is

$$(\dot{\mathrm{C}}_i)_f = \frac{\partial(\mathrm{C}_i)}{\partial t} = (\nu_i^{''} - \nu_i^{'})k_f \prod_{j=1}^{N} (\mathrm{C}_j)^{\nu_j^{'}} \tag{9}$$

For the chemical reaction proceeding in reverse direction, it is clear from eqs. (6) and (7) that the rate of reforming reactants from productos is

$$(\dot{\mathrm{C}}_i)_b = \frac{\partial(\mathrm{C}_i)}{\partial t} = (\nu_i^{'} - \nu_i^{''})k_b \prod_{j=1}^{N} (\mathrm{C}_j)^{\nu_j^{''}} \tag{10}$$

For simultaneous chenical reactions, $(\dot{\mathrm{C}}_i)$ shall represent the sum of the changes produced by individual reactions steps. Then, the reaction symbolized by eqs. (5) and (6) gives

$$(\dot{\mathrm{C}}_i) = (\nu_i^{''} - \nu_i^{'})k_f \prod_{j=1}^{N} (\mathrm{C}_j)^{\nu_j^{'}} + (\nu_i^{'} - \nu_i^{''})k_b \prod_{j=1}^{N} (\mathrm{C}_j)^{\nu_j^{''}} \tag{11}$$

At thermodynamic equilibrium

$$(\dot{\mathrm{C}}_i) = 0 \qquad (\mathrm{C}_j = (\mathrm{C}_{j,e}) \tag{12}$$

where $\mathrm{C}_{j,e}$ denotes the thermodynamic equilibrium value for species C_j. From eq. (11), then it follows that the ratio k_f/k_b satisfy the equation

$$\frac{k_f}{k_b} = \prod_{j=1}^{N} (\mathrm{C}_{j,e})^{(\nu_j^{''} - \nu_j^{'})} = K_e \tag{13}$$

Here K_e represents the usual equilibrium constant, and it is related to the ratio of the kinetics parameters k_b and k_f. The equilibrium constant can be calculated quite accurately.

The total range of change of molar concentration per unit volume of species i, is

$$(\dot{\mathrm{C}}_i)_{total} = \sum_{i=1}^{NR} (\dot{\mathrm{C}}_i) \tag{14}$$

where NR is the total number of elementary reactions taken into account. Consequently the rate of mass production of species i to be included as a source term in eq. (1) becomes

$$\dot{w}_i = M_i \cdot (\dot{\mathrm{C}}_i)_{total} \tag{15}$$

It should be noted that the expression for the chemical reaction rate, eq. (11) is strictly valid for elementary reaction steps corresponding to a complex reaction mechanism. If a global kinetic scheme is used, the exponent for molar concentrations may differ from their stoichiometric coefficients to match empirical data.

2.2 The implicit treatment of source terms

A finite volume approximation of the system of equations (1) can be written

$$\frac{\delta(\mathbf{U}\mathrm{V})_j^n}{\Delta\, t} + \left(\widetilde{\mathbf{F}}_{j+1/2}^n - \widetilde{\mathbf{F}}_{j-1/2}^n\right) = (\dot{\mathbf{W}}\mathrm{V})_j^{n+1} \tag{16}$$

where $\mathbf{U}$ is the vector of unknowns quantities, $\widetilde{\mathbf{F}}_{j+1/2}$ is the corresponding vector of numerical fluxes calculated at the cell interface $j + 1/2$ using values of the conserved quantities evaluated at cell centers at the time step n. The production or destruction of species within the cell j through chemical reactions, is represented by the vector of source terms $\dot{\mathbf{W}}$ at time step $(n + 1)$.

To separate the combined rate of change in both $\mathbf{U}$ and V so that $\delta\mathbf{U}$ may be solved directly, write

$$\delta\,(\mathbf{U}\mathrm{V})_j^n = \mathrm{V}^{n+1}\,\delta\mathbf{U}^n + \mathbf{U}^n\,\delta\mathrm{V}^n \tag{17}$$

The result of substituting eq.(17) into eq.(16) is

$$\delta\mathbf{U}_j^n + \frac{\Delta\, t}{\mathrm{V}^{n+1}}\left[\mathbf{U}_j^n\left(\frac{\delta\mathrm{V}}{\Delta t}\right)_j^n + \left(\widetilde{\mathbf{F}}_{j+1/2}^n - \widetilde{\mathbf{F}}_{j-1/2}^n\right)\right] = \dot{\mathbf{W}}_j^{n+1}\,\Delta t \tag{18}$$

Assume, now, that $\dot{\mathbf{W}}$ is linearized using a Taylor series expansion

$$\dot{\mathbf{W}}_j^{n+1} = \dot{\mathbf{W}}_j^n + \left(\frac{\partial\dot{\mathbf{W}}}{\partial\mathbf{U}}\right)_j^n \delta\mathbf{U}_j^n = \dot{\mathbf{W}}_j^n + \mathrm{A}_j^n\,\delta\mathbf{U}_j^n \tag{19}$$

where A is the Jacobian of chemical source terms respect to conserved variables. Then eq. (18) can be rewritten

$$\left[I - (\mathrm{A})_j^n\ \Delta t\right]\delta\mathbf{U}_j^n = \Delta\mathbf{U}_j^n + \dot{\mathbf{W}}_j^n\,\Delta t \tag{20}$$

where

$$\Delta\mathbf{U}_j^n = -\frac{\Delta\, t}{\mathrm{V}^{n+1}}\left[\mathbf{U}_j^n\left(\frac{\delta\mathrm{V}}{\Delta t}\right)_j^n + \left(\widetilde{\mathbf{F}}_{j+1/2}^n - \widetilde{\mathbf{F}}_{j-1/2}^n\right)\right] \tag{21}$$

Since the vector $\mathbf{U}$ has 17 components, the system of equations to be solved involves the inversion of 17×17 block matrices at each cell and time step.

The calculation of the Jacobian A is made following the technique proposed by Wilson (1992a) , which implies introducing a functional form of the source vector given by

$$\dot{\mathbf{W}}(\mathbf{U}) = \dot{\mathbf{W}}\left[\mathbf{U}, T(\mathbf{U})\right] \tag{22}$$

and the Jacobian can be calculated from

$$\mathrm{A} = \frac{\partial\dot{\mathbf{W}}}{\partial\mathbf{U}} + \frac{\partial\dot{\mathbf{W}}}{\partial T}\frac{\partial T}{\partial\mathbf{U}} \tag{23}$$

Since temporal accuracy can be affected when there is an implicit treatment of source terms as previuosly described, Leveque and Yee (1990), have stated that achieving second order accuracy in time with implicit source terms, requires a *predictor step* of the form

$$\left[I - \frac{1}{2}\left(\mathrm{A}\right)_j^n \Delta t\right] \delta\overline{\mathbf{U}}_j^n = \Delta\mathbf{U}_j^n + \dot{\mathbf{W}}_j^n \Delta t \qquad \overline{\mathbf{U}}_j^n = \mathbf{U}_j^n + \delta\overline{\mathbf{U}}_j^n \tag{24}$$

being the *corrector step*

$$\left[I - \frac{1}{2}\left(\mathrm{A}\right)_j^n \Delta t\right] \delta\widetilde{\mathbf{U}}_j^n = \Delta\overline{\mathbf{U}}_j^n + \dot{\mathbf{W}}_j^n \Delta t \qquad \mathbf{U}_j^{n+1} = \mathbf{U}_j^n + \frac{1}{2}\left(\delta\overline{\mathbf{U}}_j^n + \delta\widetilde{\mathbf{U}}_j^n\right) \tag{25}$$

Here the terms A and $\dot{\mathbf{W}}$ are evaluated using $\mathbf{U}_j^n$ on both the predictor and corrector steps.

3 NUMERICAL SIMULATIONS AND RESULTS

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 blast as it decays. Applying the numerical approach previously described to a planar starting and propagating blasts both aspects, the tendency of the initial blast wave generated by the igniter to becoming a Chapman-Jouguet phenomena and the decoupling of the reaction zone are intended to be simulated. Note that for an inviscid and adiabatic truly planar flow, the geometry which contains it becomes irrelevant.

3.1 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). In this study, the planar igniter or ignition source is materialized by a small region of length $2.5\,mm$ located at the left 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 elevated number of time steps needed ($CFL = 0.004$) to get physical meaningful answers, 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 left closed end of the detonating system. 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).

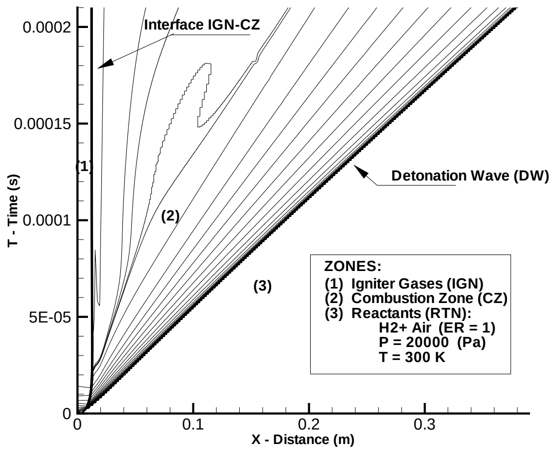


Figure 1: Computed X-T diagram of the logarithm of constant density contours - Ign. Pres.: 1.5e+06(Pa).

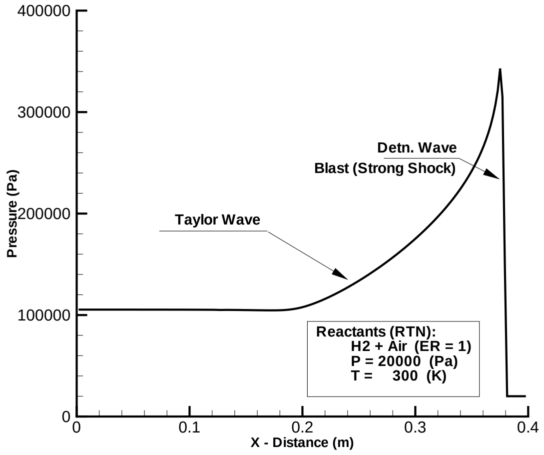


Figure 2: Computed, pressure as function of distance at flow time=2.1 e-04(s) - Ign. Press: 1.5e+06(Pa).

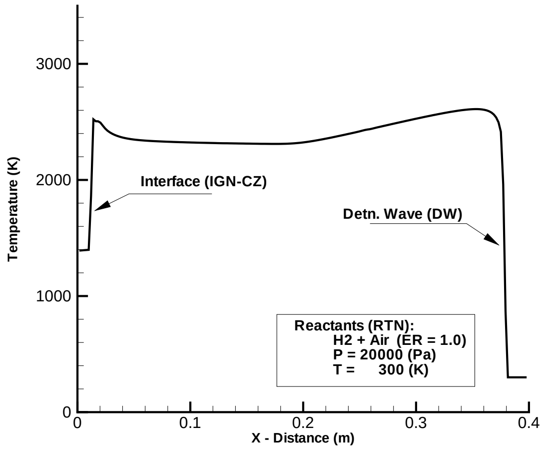


Figure 3: Computed, temperature as function of distance at flow time=2.1 e-04(s) - Ign. Press: 1.5e+06(Pa).

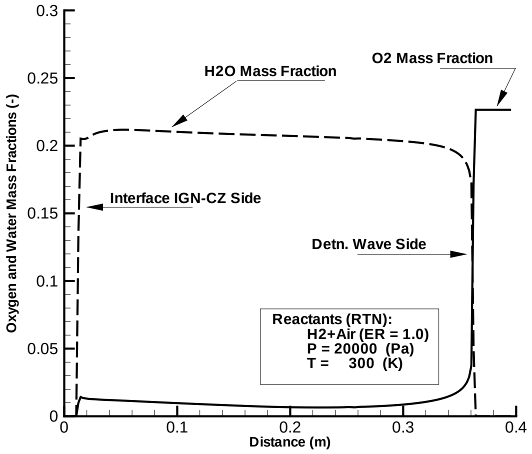


Figure 4: Computed, oxygen and water mass fractions as function of distance at flow time=2.1 e-04(s) - Ign. Press: 1.5e+06(Pa).

A close-up of the computed region near the igniter, Fig. (5), offers more details on the beginning of the detonation and on the interface separating the igniter gas from the products of the chemical reactions, which are taken place after the blast front. Notice that this interface shall not diffuse and mix, because no mechanism for diffusion is provided within the governing equations (any diffusion which might occur will only be numerical), hence, the detonation is solely due to a rapid transfer of energy from the igniter which compresses adiabatically the unburned mixture raising its temperature beyond autoignition.

As it was said, all the results presented up to now are applicable to a $H_2 + Air$ stoichiometric mixture. However, 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,

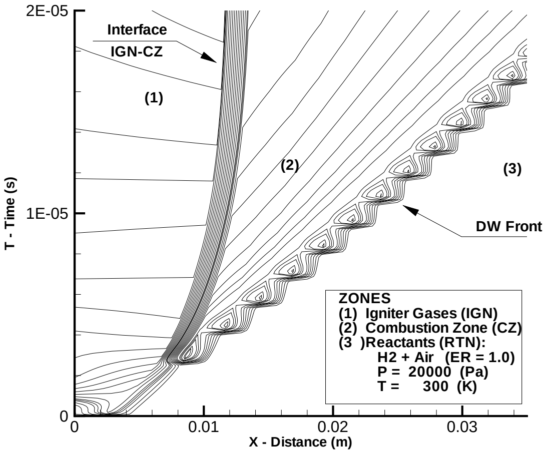


Figure 5: Computed X-T diagram in near region to the ignition source - Ign. Press.: 1.5e+06(Pa)

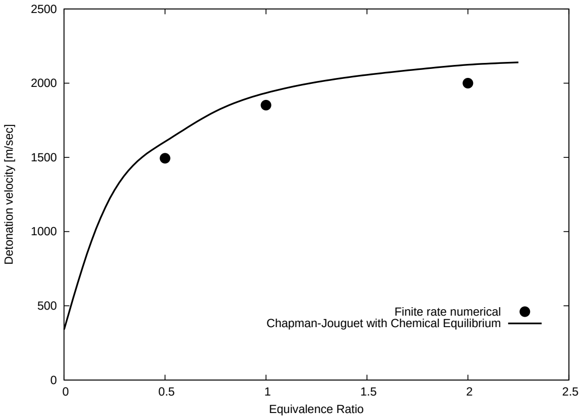


Figure 6: Comparison between detonation velocities computed using Chapman-Jouguet equilibrium and finite rates

2005; Scarpin, 2006), and using finite rate chemistry. It can be concluded from Fig.(6), that the equilibrium and finite rate calculated velocities of DWs agree satisfactorily.

When computing DWs for $ER = 0.5$ and 2.0, the pressure required at the ignition source for direct initiation must accordingly, be adjusted. Since the volume assigned to the igniter is always the same one, then the product $pressure \times igniter\ length$ can be interpreted as the energy (in terms of $Joules/m^2$), which must rapidly be delivered to the combustible medium to obtain either, an overdriven or a Chapman-Jouguet detonation. Calculations for the stoichiometric case have shown that the energy of the ignition source shall not be less than $3000\ Joules/m^2$. If to this amount an unitary value is assigned, then the ratios included in the Table 1 are applicable.

Equivalent Ratio	Energy Ratio
0.5	3.3
1.0	1.0
2.0	1.3

Table 1: Ignited energy required for detonations direct iniciation.

Apparently, the dependence on ERs of the igniter energy required for direct initiation shows the correct behavior, being in the form of a U shaped curve with the minimum around the stoichiometric mixture ($ER = 1.0$) (Kaneshige and Shepherd, 1997).

3.2 The decoupling of the reaction zone from the blast

It has been previously stated that if the igniter energy deposition is below than a certain level, let us say $3000\ Joules/m^2$ for the stoichiometric $H_2 + Air$ mixture, the combustion zone should decouple from the 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.(7) shows, in coordinates $time\ vs.\ distance$, the results obtained.

After the blast (7), a non reacting compressed region (3) develops. Although the pressure in this region (see Fig.(8)), also peaks immediately after the shock and progressively diminish

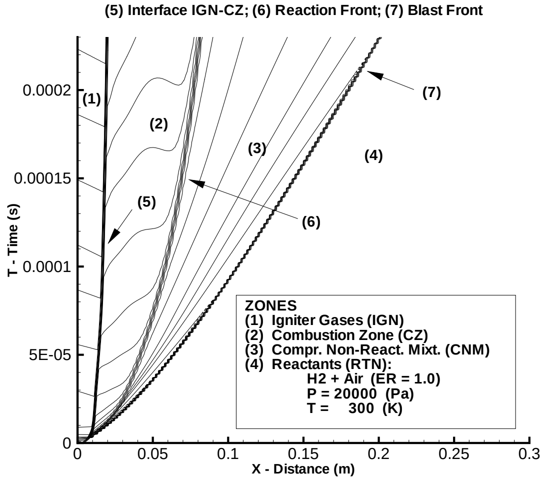


Figure 7: Computed, X-T diagram showing the combustion zone decoupled from leading blast - Ign. Press.: 1.13e+06(Pa).

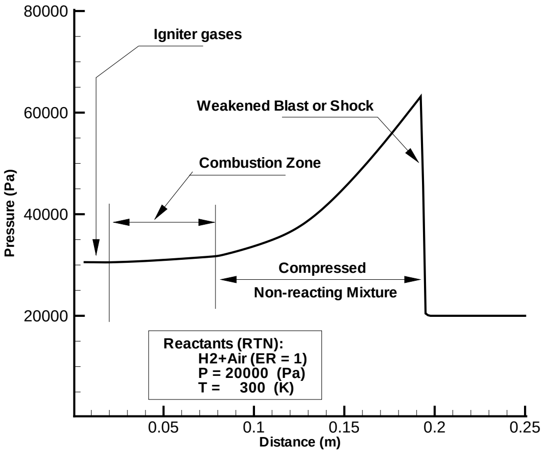
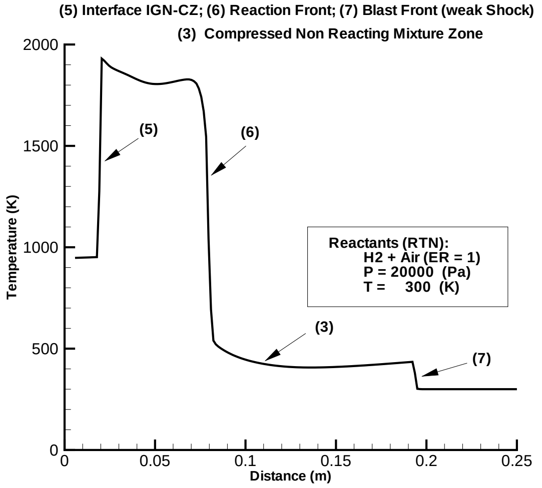


Figure 8: Computed, pressure as function of distance at flow time=2.2 e-04(s) - Combustion zone decoupled from leading blast.



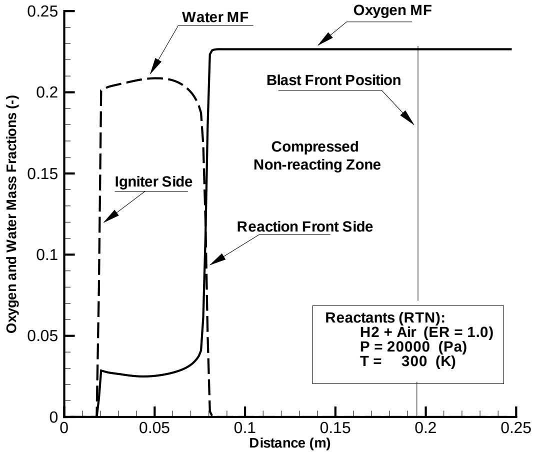


Figure 9: Computed, temperature as function of distance at flow time=2.2 e-04(s) - Combustion zone decoupled from leading blast.

Figure 10: Computed, oxygen and water mass fractions as function of distance at flow time=2.2 e-04(s) - Combustion zone decoupled from leading blast.

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.(9). 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.(10) shows computed mass fractions of oxygen and water. Both, depletion of oxygen and the formation of water corroborate locations of the combustion zone, of the associated reaction front and the limits of the expanding igniter gases. All the data used in Figs.(8), (9) and (10) have been taken from Figure (7) at a flow time of 0.22 milliseconds.

4 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 was conceived as a short length powerful driver of a shock tube that initially, 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. It shall be pointed out that in all cases computed, the interface igniter-combustion zone, always has remained confined within a small region (of few centimeters downstream of its initial position).

The main objectives accomplished, 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. Regarding initially overdriven detonations, it is proved that they decay to a Chapman-Jouguet state. When this happen, the igniter pressure has dropped from its initial maximum value to the minimum given by 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.

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