ANALYTICAL APPROACHES OF DETONATION WAVES

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DOI: 10.19062/1842-9238.2017.15.3.6

Abstract: *This paper presents some aspects regarding the gas-dynamic model of the detonation wave starting from the basic equations of mass, momentum and energy. The combustion wave speed was obtained from given initial conditions and the graphics were made for different values of energy released in the combustion process. The existence of a solution to the steady conservation laws depended on the compatibility of the solution with the dynamics of the combustion behind the wave.*

Keywords: *combustion, gas-dynamics of detonation, deflagration.*

1. INTRODUCTION

As a result of the energy release, in a combustion process can appear two types of self-propagating waves: deflagration and detonation. Deflagration waves propagate at subsonic velocities and depend not only on the initial state of the combustion mixture but also, on the boundary conditions behind the waves. Being a diffusion wave, deflagration has a velocity, proportional to the square root of the reaction rate and in stationary conditions it is defined as a flame. A detonation wave has a supersonic velocity and it can be considered as a reacting shock wave where the reactants (which are situated ahead of it) are not disturbed prior to the arrival of the detonation, remaining at their initial state. The detonation front has a transient two-dimensional structure and the flow field generated by the ignition source is responsible for the detonation formation process. Behind a strong detonation wave the flow is subsonic and the wave penetrates the reaction zone attenuating the detonation, so, a freely propagating detonation has a sonic or supersonic condition behind it.

The classical method of investigating the stability of a steady solution for self-propagating detonation wave consists of imposing small propagating multidimensional perturbations on the solution and observe if the amplitude of the perturbations grows. This assumption (of small perturbations) permits the system of equations to be linearized and integrated in order to find the unstable modes. Another method is to start with the time-dependent nonlinear equations and then integrate numerically for given initial conditions in order to see if the solution is achieved asymptotically at large time [1]. Linear stability analyses are valid only for the initial growth of the perturbations and cannot describe results far from the stability limits. The most important parameters that govern the stability of a steady detonation structure are the activation energy, E_a, the ratio of specific heats, γ, the degree of overdrive, D / D_{CJ} and the chemical heat release, Q. The detonation is unstable for high values of E_a, because small temperature perturbations result in large fluctuations in the reaction rate.

The degree of overdrive, also influences the stability of the detonation because a high degree of overdrive increases the shock temperature, T_s, having the effect of lowering the temperature sensitivity of the reaction because the exponential temperature dependence of the reaction rate depends on the ratio of activation energy and the shock temperature. Also, an increase in the heat of reaction, Q, renders the detonation more unstable, because the physical effects of the perturbations are enhanced for higher value of the heat of reaction. The possible variation of the leading shock pressure of the detonation wave as a function of time for increasing values of the activation energy is analyzed [2]. The shock pressure is normalized with respect to its value corresponding to the steady Chapman-Jouguet detonation. For a low value of the activation energy, the shock front pressure is steady.

2. BASIC EQUATIONS

For a coordinate system fixed to the wave, the basic conservation equations of mass, momentum and energy for one dimensional steady flow across a combustion wave are given by:

$$\begin{aligned} &\rho_0 u_0 = \rho_1 u_1 \\ &p_0 + \rho_0 u_0^2 = p_1 + \rho_1 u_1^2 \\ &h_0 + q + \frac{u_0^2}{2} = h_1 + \frac{u_1^2}{2} \end{aligned} \tag{1}$$

where ρ, u, p, h and q are the density, velocity, pressure, the sensible enthalpy and q is the difference between the enthalpies of formation of reactants and the products. The subscripts 0 and 1 denote the reactant and product states and the sensible enthalpy of the mixture is given by

$$h = \int_{298}^{T} c_p dT \tag{2}$$

where c_p is the specific heat of the mixture.

The existence of a steady detonation front depends on the possibility of being able to match the conditions behind a steady detonation wave to the non-steady flow in the products of chemical reaction. Planar detonation can be matched to the non-steady expansion fan behind it, being compatible with the non-steady flow of detonation products.

Starting from the caloric equation of state for the sensible enthalpy one can get the Rayleigh line and Hugoniot curve for the transition from state $(1,1)$ to state (x, y) across the combustion wave. Defining the ratios of densities and pressures as $x = \rho_0 / \rho_1 = v_1 / v_0$ and $y = p_1 / p_0$ one can write the Rayleigh line

$$y = \left(1 + \gamma_0 M_0^2\right) - \left(\gamma_0 M_0^2\right) x \tag{3}$$

and Hugoniot curve

$$y=\frac{\frac{\gamma_0+1}{\gamma_0-1}-x-2\frac{q}{p_0v_0}}{\frac{\gamma_1+1}{\gamma_1-1}x-1} \tag{4}$$

where $\gamma=c_p/c_v$ is the ratio of specific heats. The Hugoniot curve can be expressed in another form, namely

$$(y+\alpha)(x-\alpha)=\beta \tag{5}$$

where

$$\alpha=\frac{\gamma_1-1}{\gamma_1+1}$$
$$\beta=\frac{\gamma_1-1}{\gamma_1+1}\left(\frac{\gamma_0+1}{\gamma_0-1}-\frac{\gamma_1-1}{\gamma_1+1}+2\frac{q}{p_0v_0}\right) \tag{6}$$

From Rayleigh line equation we note that the velocity of the combustion wave is proportional to the square root of the slope of this line,

$$\frac{dy}{dx}=-\gamma_0M_0^2=-\frac{y-1}{1-x} \tag{7}$$

and also, the slope of the Hugoniot curve is

$$\frac{dy}{dx}=-\frac{y+\alpha}{x-\alpha} \tag{8}$$

The variation of entropy along the Hugoniot curve, in a nondimensional form $(\bar{s}=s/R)$ can be expressed as follows

$$\frac{\gamma_1+1}{\gamma_1}\left(\frac{d\bar{s}}{dx}\right)_{\substack{Hugoniot\\curve}}\left(\frac{\frac{\gamma_1-1}{\gamma_1+1}-x}{1-x}\right)x=1-M_1^2 \tag{9}$$

Depending on whether the flow behind the combustion wave is supersonic or subsonic, the downstream boundary conditions may or may not have an influence on the wave propagation speed, namely, for a subsonic flow behind the wave the back boundary condition must be satisfied by the solution of the conservation laws across the wave, but if the wave speed is also subsonic, then perturbations can propagate upstream of the wave and the upstream conditions will be altered.

According to the equation (9), if the value of x is in interval $\left(\frac{\gamma_1-1}{\gamma_1+1},1\right)$, the expression $1-M_1^2$ has the opposite sign to the entropy derivative along the Hugoniot curve. For a strong detonation, where $(d\bar{s}/dx)_{Hugoniot}<0$, it follows that $M_1<1$, that is, the downstream flow is subsonic relative to the combustion wave. When $(d\bar{s}/dx)_{Hugoniot}>0$ then $M_1>1$ and the downstream flow is supersonic, so, strong detonation and weak deflagration depend on the downstream boundary condition, but for the weak detonations and strong deflagrations (where the flow is supersonic behind the wave), the propagation of the wave cannot be influenced by the downstream boundary conditions [3, 4].

Figure 1 shows the graphics of the Rayleigh line and Hugoniot curve. The shock Hugoniot curve $(q=0)$ passes through the initial state $(1,1)$ and for finite values of q this curve lies above the shock Hugoniot curve and doesn't intersect the initial state. The intersection of the line $x=1$ and $y=1$ with the Hugoniot curve give the solutions for constant volume and constant pressure combustion. For $x\to(\gamma_1-1)/(\gamma_1+1)$ or $\rho_1/\rho_0\to(\gamma_1+1)/(\gamma_1-1)$ the denominator of the ratio (9) is zero and $y\to\infty$, that means the line of equation $x=(\gamma_1-1)/(\gamma_1+1)$ is an asymptotic line of the Hugoniot curve. The slope of the Rayleigh line can be expressed by

$$\left(\frac{dy}{dx}\right)_{\substack{Rayleigh\\line}}=-\frac{u_1^2}{p_0v_0x^2} \tag{10}$$

therefore $u_1^*=c_1^*$, that is the flow Mach number downstream of a Chapman-Jouguet detonation or deflagration, is equal to unity.

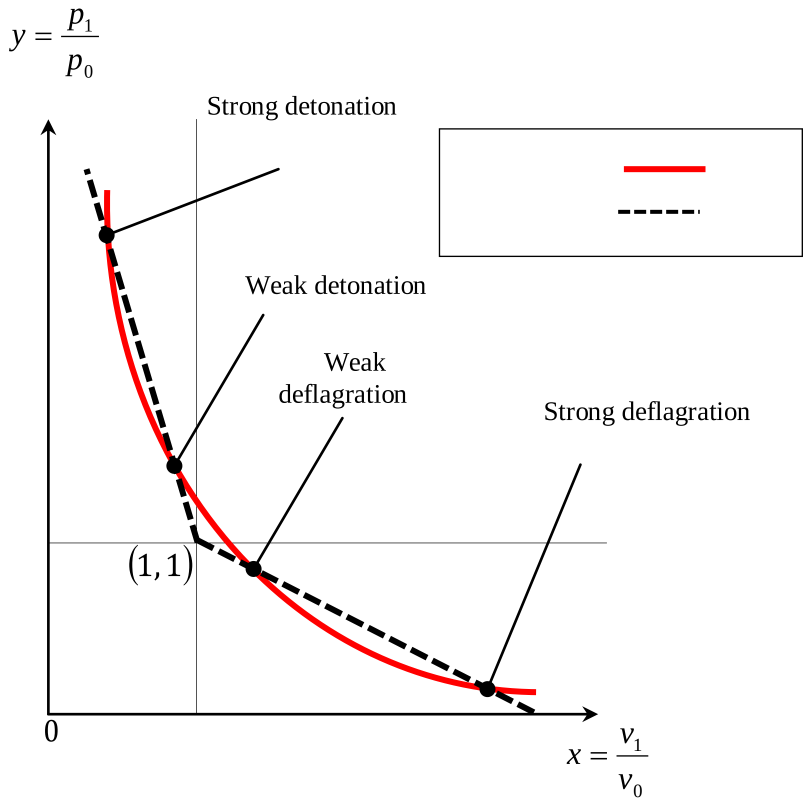


FIG. 1. The weak and strong detonation points

3. THE TANGENCY RAYLEIGH LINE AND HUGONIOT CURVE COORDINATES

For a constant chemical energy release and perfect gas assumptions it is possible to obtain the algebraic expressions relating the downstream state $(M_1, T_1, \rho_1, p_1)$to the upstream state (M_0, T_0, ρ_0, p_0).

For given initial and boundary conditions, the combustion wave speed can not be determined only from the system of conservation equations together with the equation of state, being necessary an additional relationship, which can be obtained from the Chapman-Jouguet criterion. In the point of tangency between Rayleigh line and Hugoniot curve (fig. 2) the detonation velocity is minimum and there are no solutions to the conservation equations for velocities less than this minimum value. Also, the sonic flow or minimum entropy requirement can provide a criterion for the conservation laws solution [5, 6].

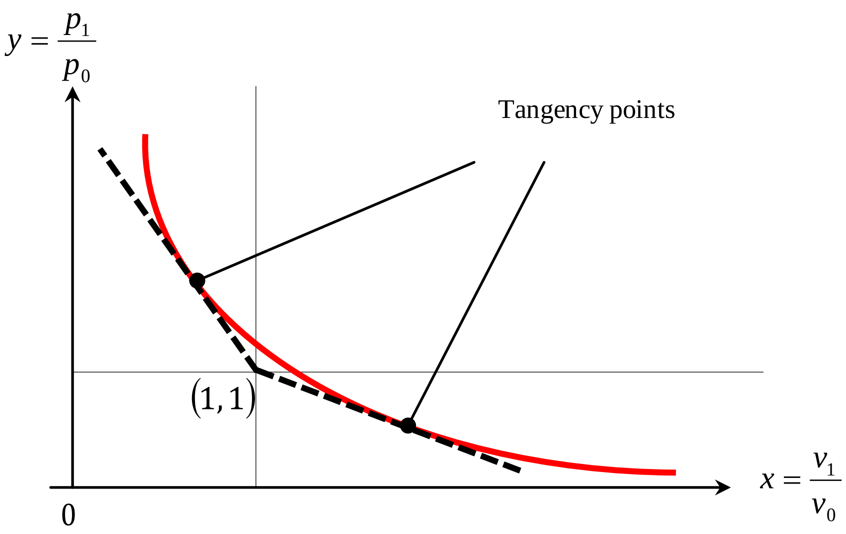


FIG. 2. The tangency solutions

Combining the equations (3) and (4) we get a quadratic equation for the specific volume ratio, $x = v_1 / v_0$,

$$x^2 - 2\frac{\gamma_1\left(\gamma_0 + \frac{1}{M_0^2}\right)}{\gamma_0(\gamma_1 + 1)}x + \frac{\gamma_1 - 1}{\gamma_1 + 1}\left[1 + 2\frac{1}{M_0^2}\left(\frac{1}{\gamma_0 - 1} + \frac{q}{c_0^2}\right)\right] = 0 \tag{11}$$

The discriminant of the above equation is

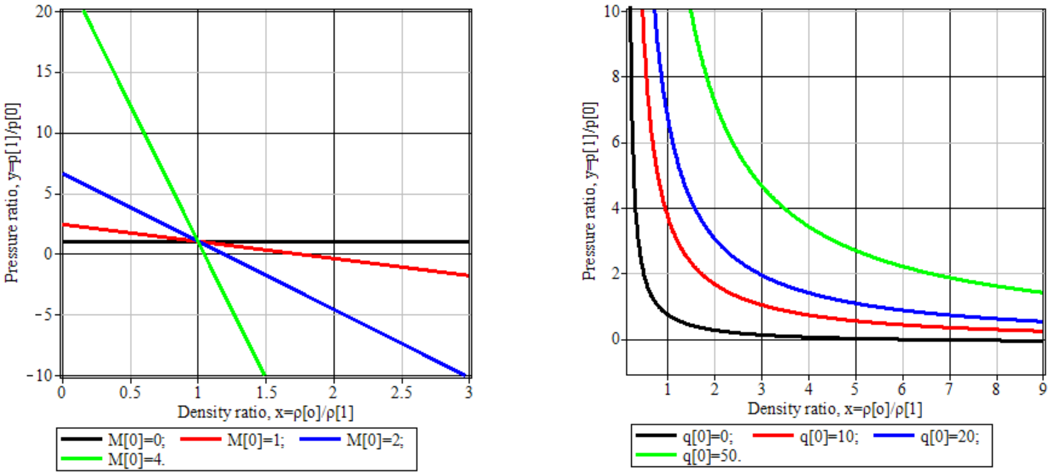
$$\Delta = \left[\frac{\gamma_1\left(\gamma_0 + \frac{1}{M_0^2}\right)}{\gamma_0(\gamma_1 + 1)}\right]^2 - \frac{\gamma_1 - 1}{\gamma_1 + 1}\left[1 + 2\frac{1}{M_0^2}\left(\frac{1}{\gamma_0 - 1} + \frac{q}{c_0^2}\right)\right] \tag{12}$$

and the solutions x_1 and x_2 can be expressed as follow

$$x_{1,2} = \left(\frac{v_1}{v_2}\right)_{1,2} = \left(\frac{\rho_0}{\rho_1}\right)_{1,2} = -\frac{\gamma_1\left(\gamma_0 + \frac{1}{M_0^2}\right)}{\gamma_0(\gamma_1 + 1)} \pm \sqrt{\Delta} \tag{13}$$

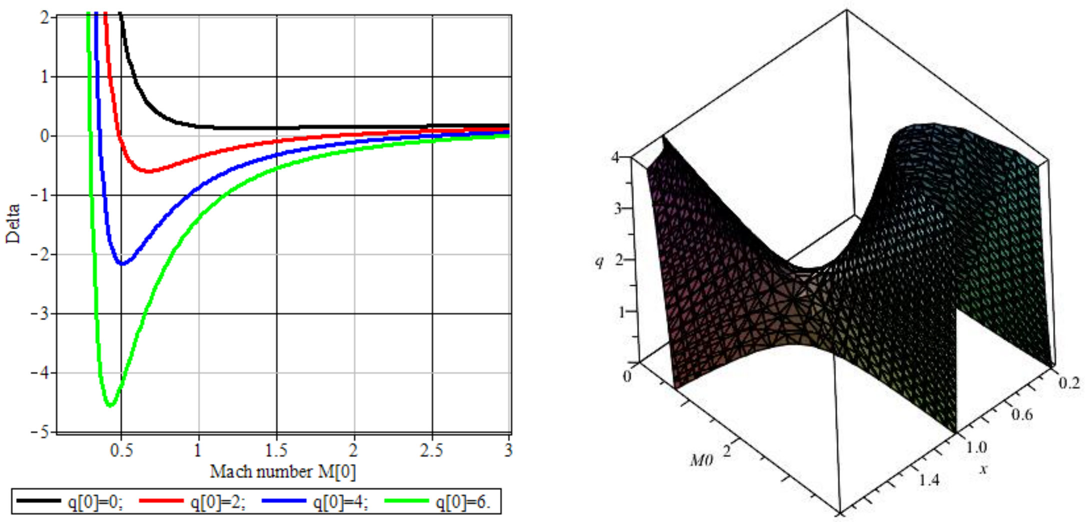
The positive sign corresponds to a weak detonation whereas the negative sign refers to a strong detonation. When the two roots coincide, we obtain the tangency solutions, which are the Chapman-Jouguet criterion. In the following picture are presented some curves for different Mach number M_0 values and for a detonable mixture corresponding to $\gamma_0 = 1.4$ and $\gamma_1 = 1.2$.

Figure 3 shows the Rayleigh lines and Hugoniot curves shapes for different values of Mach numbes M_0 and heat of reaction. Also, fig. 4 shows the discriminant function for the tangency points and the shape of solutions domain.



(a) (b)

FIG. 3. The Rayleigh lines for different values of Mach number (a) and the Hugoniot curves for different values of reaction heat



(a) (b)

FIG. 4. The discriminant of equation for tangency point solutions (a) and the domain of all possible solutions (b)

4. CONCLUSIONS

The basic theoretical aspects presented in this article permit the detonation velocity to be determined without boundary condition considerations for rear wave domain, even if their existence requires that a solution for the non-steady flow of the products match the steady boundary condition behind the Chapman-Jouguet criterion. For the planar case, the solution is continuous and the Rimann solution satisfies the sonic condition at the rear frontier of detonation, while for the cylindrical and spherical detonation there are singularities due to the infinite expansion gradient. The mathematical criterion for the sonic singularity becomes an important requirement for the choice of the correct solution from the conservation laws.

Detonation and deflagration can be analyzed using the conservation equations across the front wave and these do not require the mechanism for this transition, being necessary a model for the structure of the detonation wave, which specifies the physical and chemical processes for transforming the initial to final states.

AKNOWLEDGMENT

This work was supported by a grant of the Ministry of National Education and Romanian Space Agency, RDI Programe for Space Technology and Avanced Research - STAR, project number 174/20.07.2017.

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