

PROPAGATION OF COMBUSTION WAVES IN NOBLE-ABEL GASES

César Alejandro Quispe Gonzáles, cquispeg@lcp.inpe.br

Loreto Pizzuti, loreto@lcp.inpe.br

Fernando de Souza Costa, fernando@lcp.inpe.br

Laboratório Associado de Combustão e Propulsão, INPE

Rodovia Presidente Dutra, km 40, Cachoeira Paulista, 12630-000, SP, Brasil

Abstract. *This work analyses the propagation of combustion waves in Noble-Abel gases. The Chapman-Jouguet approach is adopted and analytical expressions are obtained for the jump conditions across the combustion waves, the Mach number and detonation velocity in the CJ point. The influence of covolume on the Rayleigh line and Hugoniot curve are considered. The results obtained for Noble-Abel gases are compared to the perfect gas solution.*

Keywords: *Detonation, Deflagration, Chapman-Jouguet, Noble-Abel, Hugoniot curve*

1. INTRODUCTION

The equation of state (EOS) for a perfect gas can be used with good accuracy at low pressures. At high pressures should be considered the effects of the volume of molecules and the forces of molecular attraction. The equation of Van der Waals was the first semi-empirical approach used to represent the behavior of real gases. In ballistics applications, the high propellant gas temperature means that inter-molecular attraction energy is small in comparison to the molecular kinetic energy (Johnston, 2005). Thus the attraction term can be removed without significant loss of accuracy, resulting in the so-called Noble-Abel (NA) equation of state, $P(v-b) = RT$, where b is called relative volume correction term (co-volume), which corresponds to about four times the volume occupied by molecules. Experimental data show that the co-volume remains approximately constant in a wide range of T and P for a given gas (Baibuz, 1985).

Combustion waves propagate in solid, liquid, gas or multiphase medium with different speeds, depending of the initial or boundary conditions. Combustion waves that propagate with subsonic velocities are called deflagrations and usually have speeds less than 1 m/s under ambient conditions and combustion waves that propagate with supersonic velocities are called detonations and usually have speeds of about 1500-2000 m/s under ambient conditions. It has been verified that the deflagration waves are approximately isobaric whereas detonation waves have high compression ratio, varying from 1.5 to 2.5 MPa.

Shepherd (2007) stated that a detonation is not just a shock wave initiated by combustion. It is a combustion wave propagating at supersonic velocity, characterized by a unique coupling between a shock wave and a zone of chemical energy release.

The classical Chapman-Jouguet (CJ) theory considers detonation waves as a discontinuity with an infinite reaction rate. Based on the CJ-theory it is possible to calculate the detonation velocity and jump conditions across the wave, for a specified gas mixture. During the Second World War, the CJ model was improved by Zeldovich, Döring and Von Neumann who considered a finite reaction rate. Their model (ZND) describes the detonation wave as a shock wave immediately followed by a reaction zone, with the thickness of this zone given by the reaction rate. The ZND theory provides the same detonation velocities and pressures than the CJ theory, the only difference between the models is the wave thickness (Zeldovich and Kompaneets, 1960; Williams, 1985; Glassman, 1996; Wingerden et al, 1999).

In real detonations the wave structure is tridimensional due to hydrodynamic instabilities. However the CJ and ZND solutions give good results for the average properties (Fickett and Davis, 2000; Kuo, 2005).

Since the pressures and temperatures attained in combustion waves can be extremely high, it is pertinent to analyse the effects of molecular volume and of the molecular attraction on the propagation characteristics of combustion waves.

Next, an analysis of the propagation of combustion waves in NA gases is presented based on the (CJ) approach (Williams, 1985; Glassman, 1996). The results are compared to the perfect gas solution.

2. THE CONSERVATION EQUATIONS

Assuming a one-dimensional steady-state flow of a NA gas, and adopting a fixed coordinate system on the combustion wave, the conservation equations of continuity, momentum and energy are given, respectively, by:

$$\rho_1 u_1 = \rho_2 u_2 = m \quad (1)$$

$$P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2 \quad (2)$$

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2} \quad (3)$$

The subscripts 1 and 2 denotes properties of reactants and products, respectively, m is the mass flow rate per unit area, P is the pressure, ρ , the density, u , the flow velocity and h is the enthalpy. The NA equations of state for reactants and products are written, respectively, as:

$$P_1(v_1 - b_1) = R_1 T_1 \quad \text{and} \quad P_2(v_2 - b_2) = R_2 T_2 \quad (4)$$

where the specific volumes are obtained from:

$$v_1 = 1/\rho_1 \quad \text{and} \quad v_2 = 1/\rho_2. \quad (5)$$

The enthalpy of a real gas (Van Wylen et al., 1994) can be obtained from:

$$dh = c_p dT + \left[v - T \left(\frac{\partial v}{\partial T} \right)_p \right] dP \quad (6)$$

and integrating for a NA gas with constant properties, it yields:

$$h_1 = h_{f,1} + c_{p,1} T_1 + b_1 P_1 \quad \text{and} \quad h_2 = h_{f,2} + c_{p,2} T_2 + b_2 P_2 \quad (7)$$

2.1. Rayleigh line

Combining Eqs. (1) and (5) it yields $u_1 = m/\rho_1 = mv_1$ and $u_2 = m/\rho_2 = mv_2$. Substituting into Eq. (2), it gives:

$$\frac{P_2 - P_1}{v_2 - v_1} = -m^2 \quad (8)$$

This equation is known as the Rayleigh line and relates the pressure variation to the specific volume variation along a combustion wave. Eq. (8) is independent of the equation of state. For a NA gas, Eq. (8) can be rewritten as:

$$\frac{P_2 - P_1}{(v_2 - b_2) - (v_1 - b_1) + (b_2 - b_1)} = -m^2 \quad (9)$$

Dividing the numerator by P_1 and the denominator by $v_1 - b_1$, defining the dimensionless variables of pressure $p = P_2/P_1$, specific volume $v = (v_2 - b_2)/(v_1 - b_1)$ and co-volume difference $b = (b_2 - b_1)/(v_1 - b_1)$, the previous equation can be rewritten as:

$$\frac{p-1}{v-1+b} = -m^2 \frac{v_1 - b_1}{P_1} = \mu \quad (10)$$

where μ is the dimensionless mass flow rate, that can be expressed in terms of the Mach number of the reactants, $M_1 = u_1/a_1$. Using the NA equation of state for the reactants, the speed of sound in real gases (Oates, 1984) is:

$$a^2 = \left(\frac{\partial P}{\partial \rho} \right)_s = \gamma v^2 \left(\frac{\partial P}{\partial T} \right)_v \left(\frac{\partial T}{\partial v} \right)_p = \gamma_1 v_1^2 \left(\frac{R_1}{v_1 - b_1} \right) \left(\frac{P_1}{R_1} \right) = \gamma_1 R_1 \frac{T_1 v_1^2}{(v_1 - b_1)^2} = \frac{\gamma_1 P_1 v_1^2}{v_1 - b_1} \quad (11)$$

Considering Eq. (11) and rearranging the expression for μ is:

$$\mu = m^2 \frac{(v_1 - b_1)}{P_1} = \frac{u_1^2}{v_1^2} \frac{(v_1 - b_1)}{P_1} \frac{\gamma_1}{\gamma_1} = \gamma_1 \frac{u_1^2}{a_1^2} = \gamma_1 M_1^2 \quad (12)$$

2.2. Rankine-Hugoniot relations

Substituting Eq. (7) into Eq. (3), the equation of energy becomes:

$$c_{p,1}T_1 + b_1P_1 + \frac{u_1^2}{2} + q = c_{p,2}T_2 + b_2P_2 + \frac{u_2^2}{2} \quad (13)$$

where $q = h_{f,2} - h_{f,1}$ is the heat of reaction. Substituting in Eq. (13) $u_1^2 = m^2 v_1^2$ and $u_2^2 = m^2 v_2^2$ from Eq. (1), $T_1 = P_1(v_1 - b_1)/R_1$ and $T_2 = P_2(v_2 - b_2)/R_2$ from Eq. (4), the expression for m^2 from Eq. (8) and dividing by $P_1(v_1 - b_1)$, using the dimensionless variables p and v , the following is obtained:

$$\frac{c_{p,2}}{R_2}pv - \frac{c_{p,1}}{R_1} + \frac{b_2}{v_1 - b_1}p - \frac{b_1}{v_1 - b_1} - \frac{1}{2}(p-1) \left[v + 1 + \frac{(b_2 + b_1)}{(v_1 - b_1)} \right] = \frac{q}{P_1(v_1 - b_1)} \quad (14)$$

Defining now the dimensionless heat flux $\alpha = q/P_1(v_1 - b_1)$, using $c_{p,1}/R_1 = \gamma_1/(\gamma_1 - 1)$ and $c_{p,2}/R_2 = \gamma_2/(\gamma_2 - 1)$, and making several algebraic manipulations, Eq. (14) reduces to:

$$pv - \left(\frac{\gamma_2 - 1}{\gamma_2 + 1} \right) (1-b)p + \left(\frac{\gamma_2 - 1}{\gamma_2 + 1} \right) v = \left(\frac{\gamma_2 - 1}{\gamma_2 + 1} \right) \left[2\alpha + \left(\frac{\gamma_1 + 1}{\gamma_1 - 1} \right) - b \right] \quad (15)$$

The canonical form of a hyperbola is $(p - p_0)(v - v_0) = K^2$, where $p = p_0$ and $v = v_0$ are horizontal and vertical asymptote, respectively. The canonical form of the hyperbole can be rewritten as:

$$pv - v_0p - p_0v + p_0v_0 = K^2 \quad (16)$$

Comparing this equation with Eq. (15) therefore yields:

$$v_0 = \frac{\gamma_2 - 1}{\gamma_2 + 1} (1-b), \quad p_0 = -\frac{\gamma_2 - 1}{\gamma_2 + 1} \quad \text{and} \quad p_0v_0 = -\left(\frac{\gamma_2 - 1}{\gamma_2 + 1} \right)^2 (1-b). \quad (17)$$

By algebraic manipulation of Eq. (15), the equation of the Hugoniot curve for NA gas is obtained:

$$\left(p + \frac{\gamma_2 - 1}{\gamma_2 + 1} \right) \left[v - \left(\frac{\gamma_2 - 1}{\gamma_2 + 1} \right) (1-b) \right] = \left(\frac{\gamma_2 - 1}{\gamma_2 + 1} \right) \left[\left(\frac{\gamma_1 + 1}{\gamma_1 - 1} \right) + 2\alpha - b - \left(\frac{\gamma_2 - 1}{\gamma_2 + 1} \right) (1-b) \right] \quad (18)$$

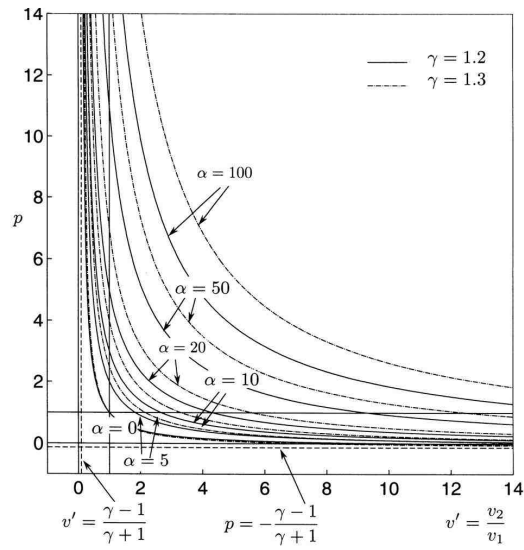
If the properties of reactants and products are constant, then Eq. (18) describes a hyperbola. If γ_2 and b_2 are function of the temperature and pressure of the products, then the hyperbola is degenerate. When $b = 0$ in Eq. (18), the Hugoniot equation of hyperbola, valid for NA gas or ideal gas with the same properties for reactants and products, is obtained:

$$\left(p + \frac{\gamma_2 - 1}{\gamma_2 + 1} \right) \left[v - \frac{\gamma_2 - 1}{\gamma_2 + 1} \right] = \left(\frac{\gamma_2 - 1}{\gamma_2 + 1} \right) \left[2\alpha + \frac{\gamma_1 + 1}{\gamma_1 - 1} - \frac{\gamma_2 - 1}{\gamma_2 + 1} \right] \quad (18.a)$$

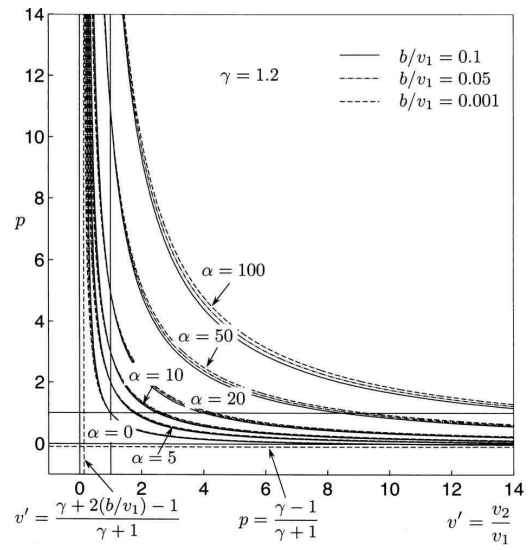
As the pressure ratio and specific volume (or velocity) ratio must be positive, they are restricted to the interval:

$$0 < p < \infty; \quad (1-b) \left(\frac{\gamma_2 - 1}{\gamma_2 + 1} \right) < v < \frac{\gamma_1 + 1}{\gamma_1 - 1} + 2\alpha - b$$

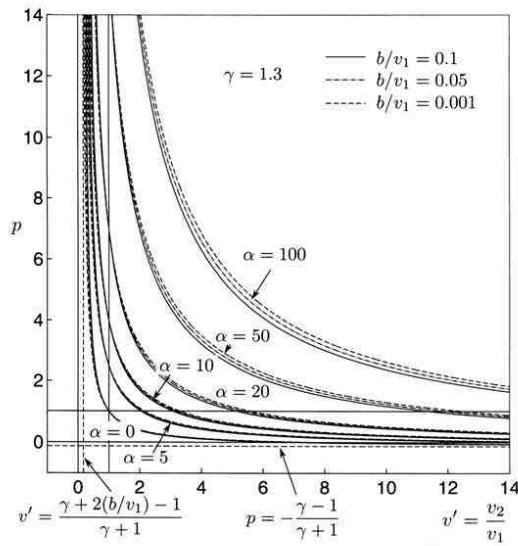
Figure 1 shows the effects of b_i , γ and α on the Hugoniot curves for NA gases.



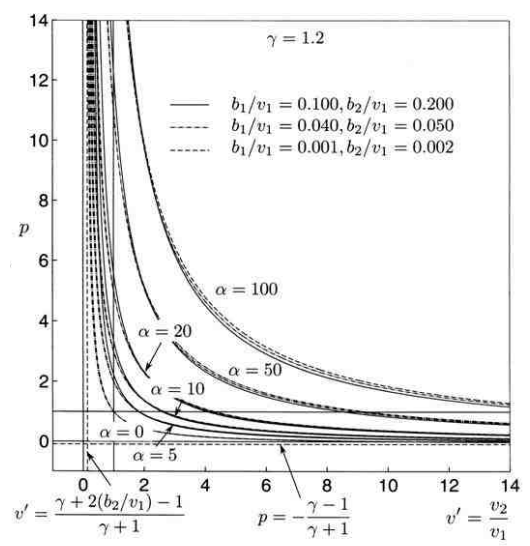
a) $\gamma_1 = \gamma_2 = \gamma$; $b_1 = b_2 = b = 0$



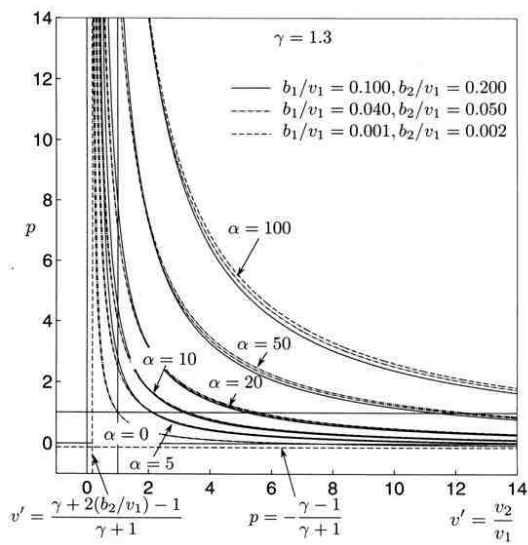
b) $\gamma_1 = \gamma_2 = 1.2$; $b_1 = b_2 = b$



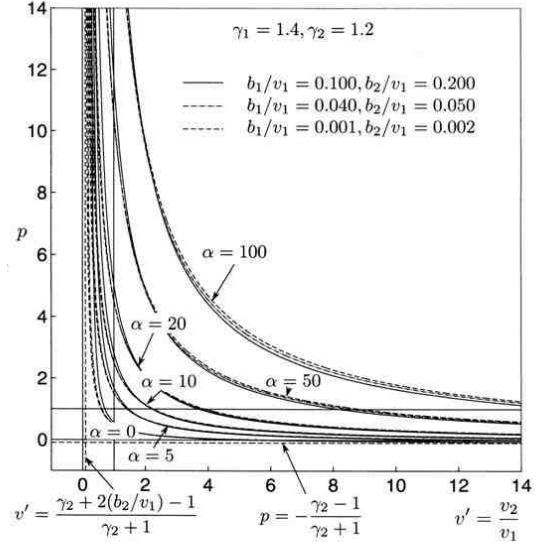
c) $\gamma_1 = \gamma_2 = 1.3$; $b_1 = b_2 = b$



d) $\gamma_1 = \gamma_2 = 1.2$; $b_1 \neq b_2$



e) $\gamma_1 = \gamma_2 = 1.3$; $b_1 \neq b_2$



f) $\gamma_1 \neq \gamma_2$; $b_1 \neq b_2$

Figure 1. Hugoniot curves for NA gases.

In figure 1, a $p - v'$ reference system is used, where:

$$p = P_2/P_1 \quad (19a)$$

$$v = \frac{v_2 - b_2}{v_1 - b_1} = \frac{v_2/v_1 - b_2/v_1}{1 - b_1/v_1} = \frac{v' - b_2/v_1}{1 - b_1/v_1} \Rightarrow v' = v \left(1 - \frac{b_1}{v_1} \right) + \frac{b_2}{v_1} \quad (19b)$$

and the co-volume relative difference is:

$$b = \frac{b_2 - b_1}{v_1 - b_1} = \frac{b_2/v_1 - b_1/v_1}{1 - b_1/v_1} \quad (19c)$$

2.3. Properties of Chapman-Jouguet waves

When the Rayleigh line is tangential to the Hugoniot curve, the upper and lower CJ points are determined. In the CJ points the Mach number of the products is unitary, $M_2 = 1$. This result is independent of the used equation of state, as shown by Kuo (2005). The Rayleigh line, Eq. (9), for a NA gas, can be written as:

$$\frac{dp}{dv} = -\mu = \frac{p-1}{v-1+b} \quad (20)$$

Differentiating Eq. (18.a) yields:

$$\frac{dp}{dv} = -\frac{(\gamma_2 + 1)p + (\gamma_2 - 1)}{(\gamma_2 + 1)v - (\gamma_2 - 1)(1-b)} \quad (21)$$

Equating the derivatives (20) and (21) and solving, expressions for p and v as functions of each other can be obtained:

$$p = \frac{v}{v(\gamma_2 + 1) + \gamma_2(b-1)} \quad (22)$$

$$v = \frac{\gamma_2(1-b)p}{(\gamma_2 + 1)p - 1} \quad (23)$$

These expressions are valid for the upper CJ point (detonations) and lower CJ point (deflagrations). It can be seen that, for p and v be positive, it is necessary that:

$$v > \frac{\gamma_2(1-b)}{\gamma_2 + 1} \quad \text{and} \quad p > \frac{1}{\gamma_2 + 1}$$

Substituting v and p from Eq. (22) and Eq. (23) into Eq. (15), p and v , as function of the parameters α , γ_1 and γ_2 can be calculated:

$$p_{\pm} = \frac{(\gamma_2 - 1)}{(1-b)} \left(\alpha + \frac{1}{\gamma_1 - 1} \right) \left\{ 1 \pm \left[1 - \frac{(1-b) \left(2\alpha + \frac{\gamma_1 + 1}{\gamma_1 - 1} - b \right)}{(\gamma_2^2 - 1) \left(\alpha + \frac{1}{\gamma_1 - 1} \right)^2} \right]^{1/2} \right\} \quad (24)$$

$$v_{\pm} = \frac{(\gamma_2 - 1)}{\gamma_2} \left(\alpha + \frac{1}{\gamma_1 - 1} - b \right) \left\{ 1 \mp \left[1 - \frac{\gamma_2^2 (1 - b) \left(2\alpha + \frac{\gamma_1 + 1}{\gamma_1 - 1} - b \right)}{(\gamma_2^2 - 1) \left(\alpha + \frac{1}{\gamma_1 - 1} - b \right)^2} \right]^{1/2} \right\} \quad (25)$$

In Eq. (24) and Eq. (25), higher signs correspond to a detonation and lower signs correspond to a deflagration. When $b_1 = b_2$ and $\gamma_1 = \gamma_2 = \gamma$, then Eq. (24) and Eq. (25) simplify and become valid for a perfect gas with constant properties, resulting in:

$$p_{\pm} = 1 + \alpha(\gamma - 1) \left\{ 1 \pm \left[1 + \frac{2\gamma}{\alpha(\gamma^2 - 1)} \right]^{1/2} \right\} \quad (26)$$

$$v_{\pm} = 1 + \frac{\gamma - 1}{\gamma} \alpha \left\{ 1 \mp \left[1 + \frac{2\gamma}{\alpha(\gamma^2 - 1)} \right]^{1/2} \right\} \quad (27)$$

Equation (12) gives an expression for M_1^2 as a function of p and v :

$$M_{1\pm}^2 = -\frac{\mu_{\pm}}{\gamma_1} = -\frac{1}{\gamma_1} \left(\frac{p_{\pm} - 1}{v_{\pm} - 1 + b} \right) \quad (28)$$

Mach numbers in the reactants for detonations and deflagrations are obtained by substituting the expressions for p_{\pm} and v_{\pm} in Eq. (28). The temperature ratio along a combustion wave can be calculated by:

$$T_{\pm} = T_{2\pm} / T_{1\pm} = (R_1 / R_2) p_{\pm} v_{\pm}. \quad (29)$$

Figure 2 shows the dependence of the properties of the combustion waves upon the dimensionless heat-release parameter α in NA gases, for several cases. In Tab. 1 the parameter values of some alkanes, used to draw Fig. (2.f), are given.

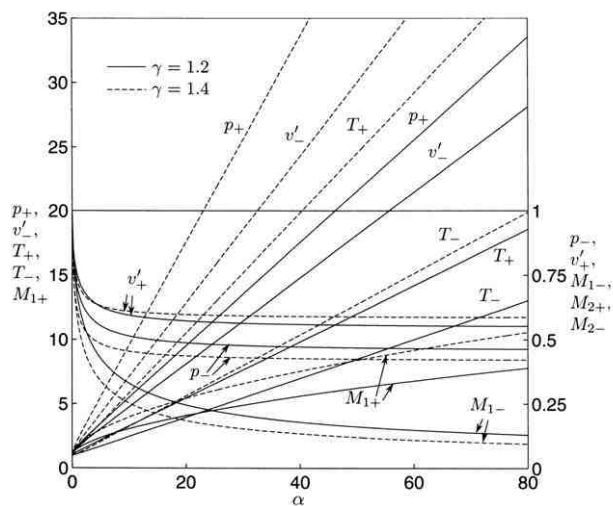
Table 1 – Parameter values of the some alkanes.

Properties	γ_1	γ_2	R_1 (J/kg.K)	R_2 (J/kg.K)	b_1/v_1	b_2/v_1
CH ₄	1,389	1,251	300,80	303,10	0,002921	0,002678
C ₃ H ₈	1,368	1,252	282,12	296,30	0,00308	0,002855
iso-C ₈ H ₁₈	1,354	1,252	274,75	293,47	0,00318	0,002932

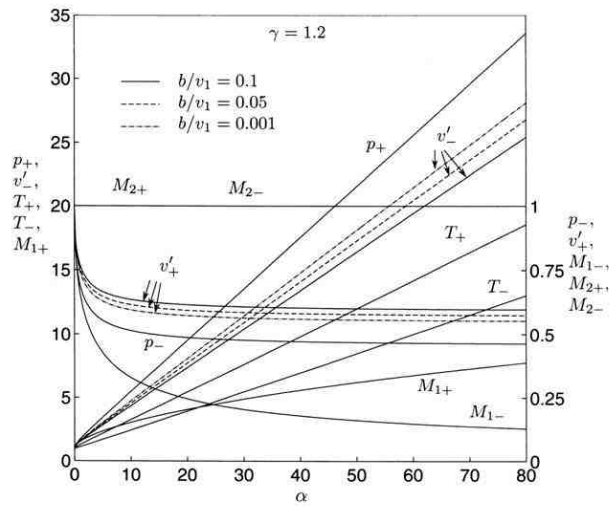
2.4. Temperatures and stagnation conditions

The stagnation temperature, T_{0i} , for a NA gas, considering $\hat{b}_i = b_i / v_i$, $i=1,2$, is obtained from:

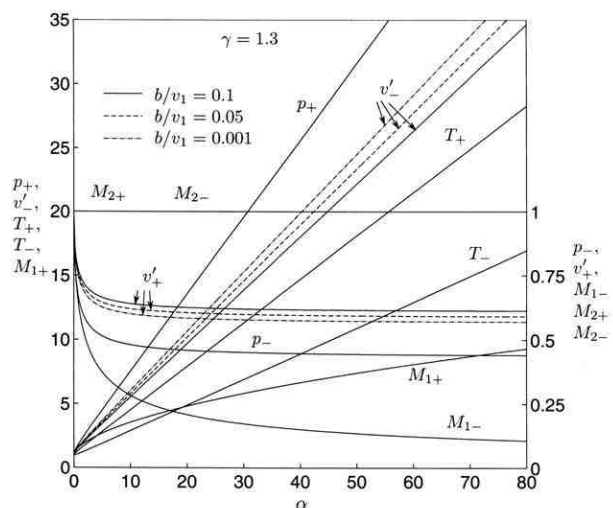
$$\frac{T_{0,i}}{T_i} = 1 + \frac{(\gamma_i - 1)}{2(1 - \hat{b}_i)^2} M_i^2 + \frac{\hat{b}_i(\gamma_i - 1)}{\gamma_i(1 - \hat{b}_i)} \left(1 - \frac{P_{0,i}}{P_i} \right) \quad (30)$$



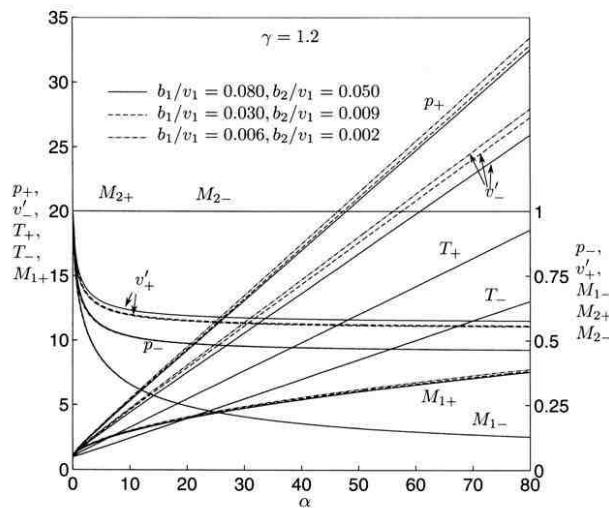
a) $\gamma_1 = \gamma_2 = \gamma$; $b_1 = b_2 = b = 0$



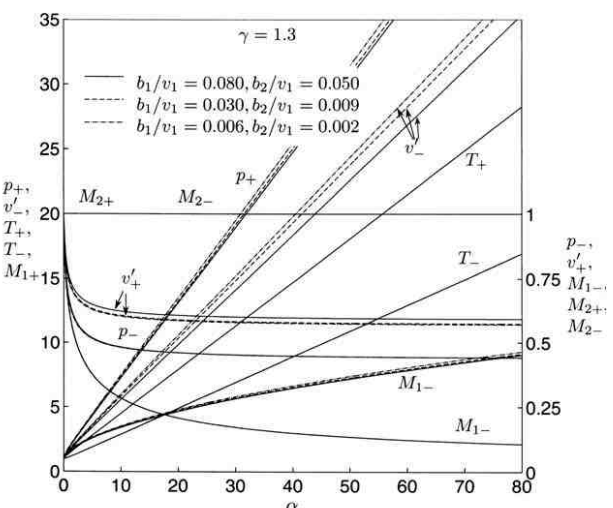
b) $\gamma_1 = \gamma_2 = 1.2$; $b_1 = b_2 = b$



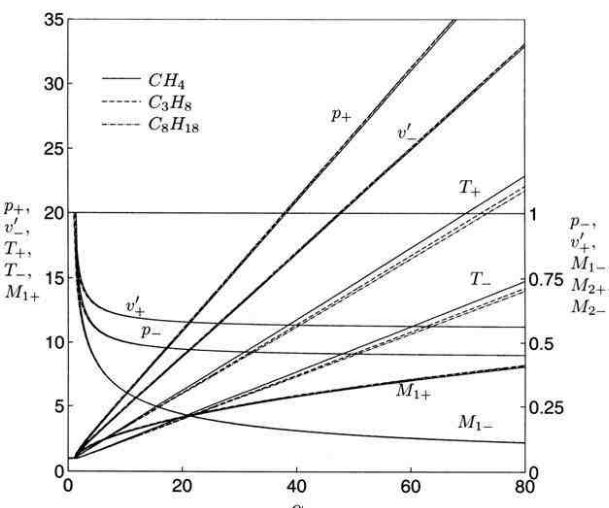
c) $\gamma_1 = \gamma_2 = 1.3$; $b_1 = b_2 = b$



d) $\gamma_1 = \gamma_2 = 1.2$; $b_1 \neq b_2$



e) $\gamma_1 = \gamma_2 = 1.3$; $b_1 \neq b_2$



f) combustion of alkanes in air

Figure 2. Properties of combustion waves in NA gases versus heat release, α .

For an isentropic process in a NA gas it can be shown that $P_{0,i}/P_i = (T_{0,i}/T_i)^{\frac{\gamma_i}{\gamma_i-1}}$. Therefore, Eq. (30) can be rewritten as:

$$\frac{T_{0,i}}{T_i} = 1 + \frac{(\gamma_i - 1)}{2(1 - \hat{b}_i)^2} M_i^2 + \frac{\hat{b}_i(\gamma_i - 1)}{\gamma_i(1 - \hat{b}_i)} \left[1 - \left(\frac{T_{0,i}}{T_i} \right)^{\frac{\gamma_i}{\gamma_i-1}} \right] \quad (31)$$

The ratio of stagnation temperatures of a NA gas and a perfect gas is:

$$\frac{T_{0,i,NA}}{T_{0,i,PG}} = \frac{1 + \frac{(\gamma_i - 1)}{2(1 - \hat{b}_i)^2} M_i^2 + \frac{\hat{b}_i(\gamma_i - 1)}{\gamma_i(1 - \hat{b}_i)} \left[1 - \left(\frac{T_{0,i}}{T_i} \right)^{\frac{\gamma_i}{\gamma_i-1}} \right]}{1 + \frac{(\gamma_i - 1)}{2} M_i^2} \quad (32)$$

Figure 3 compares the behavior of the stagnation temperature and pressure for NA and perfect gases.

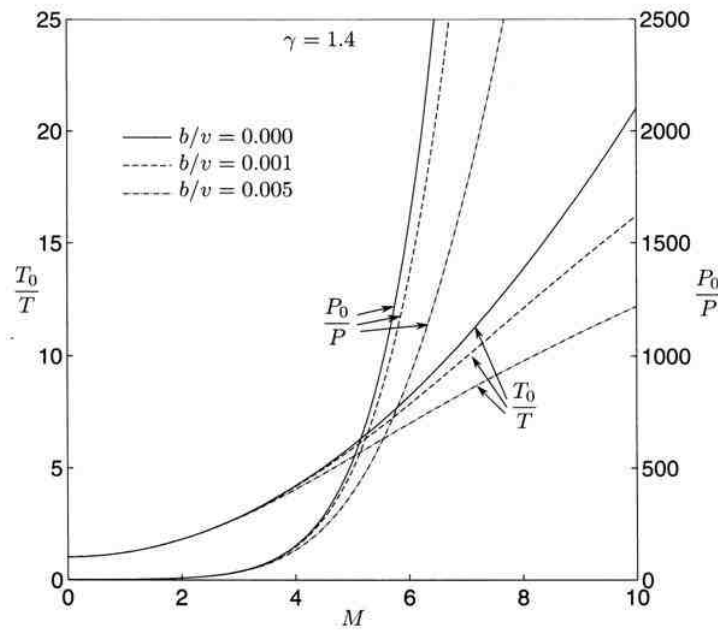


Figure 3 – Stagnation to static temperature and pressure ratio for NA gases, dotted line, and perfect gases, solid line. ($\gamma_1 = \gamma_2 = 1.4$ and $b_1 = b_2 = b$).

The stagnation temperature after CJ combustion wave ($M_2 = 1$) is obtained from:

$$\left(\frac{T_{0,2}}{T_2} \right)_{CJ} = 1 + \frac{\gamma_2 - 1}{2(1 - \hat{b}_2)^2} + \frac{\hat{b}_2(\gamma_2 - 1)}{\gamma_2(1 - \hat{b}_2)} \left[1 - \left(\frac{T_{0,2}}{T_2} \right)_{CJ}^{\frac{\gamma_2}{\gamma_2-1}} \right] \quad (33)$$

Once known the stagnation temperatures, their ratio can be calculated. Given the parameters (b_i , γ_i , R_i and α) of reactants and products, the pressure, specific volume and temperature ratios, Mach numbers and stagnation conditions in the CJ combustion waves (deflagrations and detonations) in NA gases can be calculated.

3. DISCUSSIONS

The influences of b_i , γ_i and α on the propagation of combustion waves in NA gases are discussed next.

a) Influence of γ_i

The influence of γ_i in the Hugoniot diagram for NA gases is similar to that observed in perfect gases (Williams, 1985). The higher the value of γ_i , the further the hyperbola vertex moves away from its center, as shown in Fig. (1a). This means that the quantity of the released heat in the reaction increases with the value of γ_i .

The influence of γ_i on the properties of the CJ combustion waves can be seen in Fig. (2a). For the CJ detonation waves, increasing γ_i , the pressure ratio p_+ , temperature ratio T_+ and the initial Mach number, M_{1+} also increases whereas the specific volume ratio, v_+ , presents a particular behavior, since it initially decreases until a certain value, and then reverses its trend. For the CJ deflagration waves, the pressure ratio p_- and the initial Mach number M_{1-} decreases, while the specific volume ratio v_- and temperature ratio T_- increase when γ_i increases. M_2 doesn't change with γ_i for both detonation and deflagration waves.

b) Influence of co-volumes

When the co-volumes $b_1 = b_2 = 0$ and $\gamma = \text{const}$, then the relative co-volume is $b = 0$ and NA gas behaves as a perfect gas. In this case, the Hugoniot diagram and the properties of the CJ combustion waves are shown in Fig. (1a) and Fig. (2a) and they are identical to the curves obtained by Williams (1985).

According to Eq. (11) the speed of sound in NA gas increases as the co-volume b_i increases. The speed of sound in a NA gas is higher than the speed of sound in a perfect gas with the same properties and under the same thermodynamic conditions. Furthermore, increasing the co-volume value, the stagnation properties, T_0 and P_0 , decrease, considering the same conditions of T and P , as shown in Fig. (3).

Case $b_1 = b_2 = \text{const}$ and different from zero and $\gamma = \text{const}$:

In this case the relative co-volume b is zero. The branches of the Hugoniot hyperbole with different values of co-volume, but with the same value of α , have a common point of intersection that is located on the vertical line $v' = 1$ as shown in Fig. (1b). In the detonations branch, the hyperbola moves to the right as the co-volume value increases. In the deflagration branch, the curve moves down increasing the co-volume value. It can be seen that the vertex of the Hugoniot curve moves away from the center point when the co-volume value decreases.

The pressure ratio, the initial Mach number and the temperature ratio for both detonation and deflagration waves are independent of b according to Eq. (24), Eq. (28) and Eq. (29) respectively. The specific volume ratio instead, increases with the co-volume value according to Eq. (25) and Eq. (19b) as shown in Fig. (2b) and Fig. (2c) in case of detonations and decreases with the co-volume value in case of deflagrations with the trends observed in Fig. (2b).

Case $b_1 > b_2$, different from zero and $\gamma = \text{const}$.

This is the most common case since the reagents molecules are generally larger than that of the products, provides the relative co-volume $b < 0$ and it is shown in the Fig. (1c). It is observed that for different values of b , the Hugoniot curves are crossing a common point located to the right of the vertical line $v' = 1$. For the detonation branch this common point moves to the right increasing the co-volume value as in the deflagration branch it moves down. In addition the vertex of the Hugoniot curve moves farther from the center point when the co-volume value decreases.

When both the co-volume values increase, the properties of the detonation waves p_+ and M_{1+} decrease, while v'_+ increases. The increasing of T_+ instead, is non-significant according to Fig. (2d). In the case of deflagration waves, increasing both the co-volume values, v'_- shows a significant decrease, the temperature ratio T_- and pressure ratio p_- increase while the initial Mach number M_{1-} decreases in an imperceptible manner.

Case $b_1 < b_2$ different from zero and $\gamma = \text{const}$.

In this case, the relative co-volume is positive, $b > 0$ and for different values of b , the Hugoniot curves are crossing a common point located to the left of the vertical line $v' = 1$. Increasing the co-volume, the detonation branch moves to the right and the deflagration branch moves down. Again, decreasing the co-volume, the vertex of the Hugoniot curve moves farther from the center point.

With the increase of the co-volume, all properties of the detonation waves showed a significant increase except for the temperature ratio T_+ . For deflagration waves, all properties decrease, but only the specific volume ratio v'_- shows a significant decrease.

Real case of combustion waves for alkanes in air.

Properties of combustion waves in Noble-Abel gases for combustion of some alkanes with air are shown in Fig. (2f). It is observed that for the three cases under review $b_1 > b_2$ and $\gamma_1 > \gamma_2$, according to Table 1, as the size of the reactants molecules is greater than that of the products, it means that the reactants are able to store a higher quantity of energy than the products. For detonation waves, the pressure ratio p_+ and initial Mach number M_{1+} increases as the co-volume values increase, while the temperature ratio T_+ decreases. The specific volume ratio v'_+ shows little changes only for

small α values. For deflagration waves, increasing the co-volume values, the pressure ratio p_+ and the initial Mach number M_1 show a significant slight decrease only for small values of α , while the specific volume ratio increases and the temperature ratio T_+ decreases in a significant manner.

c) Influence of α

The vertex of the Hugoniot curve moves farther from its center when increasing the value of α . This causes an increase in the pressure and specific volume ratios, as shown in Fig. (1).

For detonation waves, the pressure ratio p_+ , the temperature ratio T_+ and the initial Mach number M_1 increase, while the specific volume ratio v'_+ decreases fast for small values of α and then remains almost constant when α increases, as may be seen in Fig. (2). For deflagration waves, the specific volume ratio v'_- and the temperature ratio T_+ increase with the increase of α , while the pressure ratio p_+ and the initial Mach number M_1 show a fast decrease for small values of α and then remain almost constant, as observed in Fig. (2).

For a reaction where the properties γ_1, b_1 of the reactants and γ_2, b_2 of the products are different, a minimum quantity of heat, α_{min} , is required to start the reaction as is shown in Figs. (1.f) and (2.f). This quantity of minimum dimensionless heat depends on the properties of reagents γ_1, b_1 and products γ_2, b_2 , and can be found from the Eq. (24) making the discriminant equal to zero, which provides:

$$\alpha_{min} = \frac{(1-b)}{(\gamma_2-1)} - \frac{1}{\gamma_1-1} \quad (34)$$

4. CONCLUSIONS

This paper presented a simplified description of the propagation of combustion waves in NA gases, considering the CJ approach. Analytical expressions for the properties along combustion waves were obtained in terms of dimensionless volumes and co-volume differences, thus allowing an easy analysis and comparison between NA and perfect gases. It was verified that the effects of variations in co-volumes and specific heat ratios along combustion waves in NA gases can be significant.

5. REFERENCES

- Baibuz, V. F., Zitserman, V. Yu., Golubushkin, L. M., and Malyshev, I. G., "The Covolume and Equation of State of High-Temperature Real Gases", Institute of High Temperatures, Academy of Sciences of the USSR, Moscow, 1985.
- Fickett, W., Davis, W.C., "Detonation Theory and Experiment", Dover Publications, 2000.
- Glassman, I., "Combustion", 3rd ed., Academic Press, 1996.
- Johnston, I.A., "The Nobel-Abel Equation of State: Thermodynamic Derivations for Ballistics Modeling" Defense Science and Technology Organization. Australian Government Department of Defense, Edinburgh, 2005.
- Kuo, K.K., "Principles of Combustion", John Wiley & Sons, New York, 2005.
- Oates, G. C., "Aerothermodynamics of Gas Turbine and Rocket Propulsion" American Institute of Aeronautics and Astronautics, New York, 1984.
- Shepherd, J., "Detonation Waves", I Escola de Combustão, Rede Nacional de Combustão, Florianópolis-Brasil, 2007, http://www.redenacionaldecombustao.org/escoladecombustao/arquivos/EDC2007/combustao/Joseph_Shepherd_09-Detonation_Waves.pdf Acess in July, 22nd, 2009.
- Van Wylen, G.J., Sonntag R.E., Borgnakke, C., "Fundamentals of Classical Thermodynamics", 4th ed., John Wiley and Sons, New York, USA, 1994.
- Wingerden, K.V., Bjerketved, T.D., Bakke, J.R., "Detonation in Pipes and in the Open", Porsgrunn-Norway, Christian Michelsen Research and GexCon, 1999, <http://www.safetynet.de/Publications/articles/CMRNov99.pdf> Access in July 21st, 2009.
- Williams, F. A., "Combustion Theory", Perseus Books Publishing, Massachusetts, 1985.
- Zeldovich, J. B., Kompaneets, A. S., "Theory of Detonation", 1960, New York: Academic Press.

5. RESPONSABILITY NOTICE

The authors are the only responsible for the printed material included in this paper. All rights reserved.