# AN ANALYTICAL MODEL FOR THE STRUCTURE OF THE DETONATION WAVES. APPLICATION FOR HYPERSONIC PROPULSION

CORNELIU BERBENTE , MARIUS BREBENEL, SORIN BERBENTE

*Abstract.* The gas flow field within an 1D normal detonation wave at variable specific heats and viscosity with temperature is considered. Such detonation waves appear in the so called air-breathing scramjet engines used at hypersonic speed in order to avoid the dissociation by slowing down the flow to subsonic speeds. The obtained waves are possible by adjusting the mass flow to Chapman-Jouguet rates when the strong detonation and weak detonation point coincide. At some distance from the wave, the flow is isoenergetic (constant total enthalpy) as there is no time for heat transfer. Examples of application for combustion of Hydrogen in air with attention on NO formation when air is in excess are given.

*Key words:* Chapman-Jouguet mass rate, equivalent Mach number, isoenergetic flow

## 1. INTRODUCTION

The supersonic combustion represents a solution to avoid the dissociation at hypersonic Mach numbers thus reducing the energy consumption and atmosphere pollution [1,2,4]. At very high Mach numbers ($M > 5$) decreasing the flow velocity to subsonic regimes will lead to high temperatures; then, by adding heat, the dissociation appears at large extent. In this paper, attention is paid to analytical work out of the basic flow equations in order to obtain simple and compact formulas for the main flow parameters. In this way the variation of thermodynamic functions with temperature [7,8] and the change of composition connected with the chemical reactions [1] is more completely described, by introducing the effects of air excess and dissociation, to evaluate its influence on engine efficiency. One interesting and important result obtained analytically is that the Mach number behind the Chapman-Jouguet combustion wave is larger then 1; on the other hand, the equivalent Mach number behind this wave, denoted by $M_e$, is critical.

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## 2. CHAPMAN-JOUGUET COMBUSTION WAVES

Before studying the waves' structure, one needs to adjust the flow mass rate to the Chapman-Jouguet conditions.

To this aim, a global calculation is done by using the conservation laws in a simpler form [1, 3].

The atmospheric air enters at high supersonic speeds (Mach number $M_H \geq 5$) in the engine inlet, as in Fig. 1. After a compression through the oblique shock waves OS and ST, the liquid hydrogen is injected and vaporized to obtain a premixed fuel (hydrogen) and oxidizer (air). The combustion of the gas mixture is initiated and a detonation wave occurs. According to the physical model of Zeldovich-Neumann-Doering [5], the detonation wave consists of a shock wave increasing the mixture temperature and a deflagration wave (flame). The air velocity, density, pressure and temperature are denoted by $V_H, \rho_H, p_H, T_H$ at the flight altitude *H*. The oblique waves are stabilized by a narrowing downstream area. One can also use the temperature rise due to these waves to provide the necessary heat for vaporizing the injected hydrogen. Thus, by adjusting the angles $\omega_{in}$ and $\omega_s$ (Fig. 1), one could take the same conditions in section 1 as at entrance, except for velocity and Mach number, which are a little smaller.

The viscous effects are concentrated in the shock wave, whereas the thermal conductivity effects are concentrated in the flame. These two waves are then the only entropy sources.

Assuming a one-dimensional steady and inviscid flow with no heat transfer, the equations modelling the normal shock waves without structure are:

$$\rho_1 V_1 = \rho_2 V_2 \quad \text{(mass conservation)} \tag{1}$$

$$p_1 + \rho_1 V_1^2 = p_2 + \rho_2 V_2^2 \quad \text{(momentum conservation)} \tag{2}$$

$$h_1(T_1) + \frac{1}{2} V_1^2 = h_2(T_2) + \frac{1}{2} V_2^2 \quad \text{(energy conservation)} \tag{3}$$

where $V_j, \rho_j, p_j, T_j$, $j = (1,2)$ are velocities, densities, pressures and temperatures respectively. The enthalpy $h$ of an ideal gas is a function of the temperature *T* only, and can be written as:

$$h(T) = h(T_{ref}) + \int_{T_{ref}}^{T} c_p(T) \cdot \mathrm{d}T \tag{4}$$

$T_{ref} = 298.15\,\mathrm{K}$ being a reference temperature and $c_p(T)$ the specific heat at constant pressure. The specific heat of reaction, denoted by *q*, is the enthalpy difference at the initial temperature.

Now, one introduces an average specific heat $c_{pm}^{(2)}(T_1,T_2)$ defined by:

$$c_{pm}^{(2)}(T_1,T_2)=\frac{1}{T_2-T_1}\int_{T_1}^{T_2} c_p(T)\cdot \mathrm{d}T \tag{5}$$

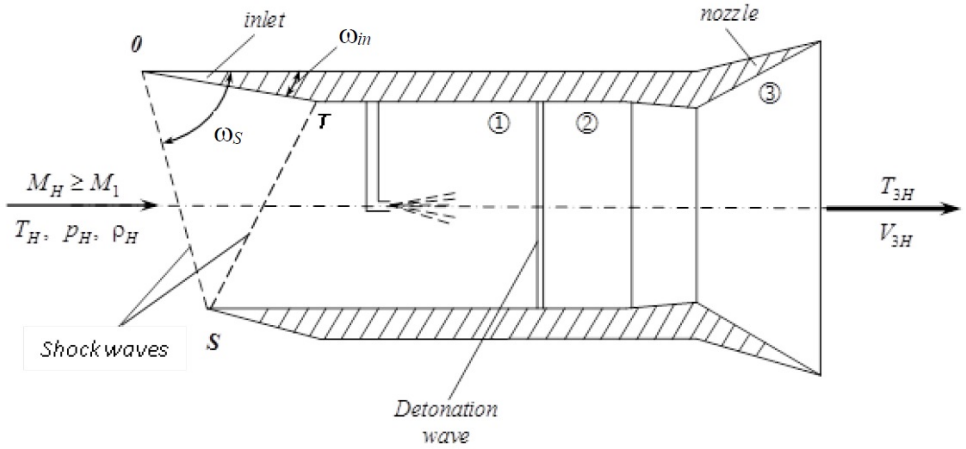


Fig. 1 – Ramjet engine configuration.

Using this, the energy equation for the combustion wave can be written in the form [7]:

$$c_{pm}^{(2)}\cdot T_1+\frac{1}{2}V_1^2+q(T_1)=c_{pm}^{(2)}\cdot T_2+\frac{1}{2}V_2^2\ ;\quad q(T_1)=h_1(T_1)-h_2(T_1) \tag{6}$$

After some algebra, one can eliminate the velocity from the above equations, to obtain:

$$\begin{gathered} p_r=1+\bar{m}\left(1-\tau_r\right)\ ;\quad p_r=p_2/p_1\ ,\quad \tau_r=\rho_1/\rho_2 \\ T_r=\frac{R_1}{R_2}p_r\tau_r\ ;\quad T_r=T_2/T_1\ ;\quad \bar{m}=k_1M_1^2 \end{gathered} \tag{7}$$

where $R_1$, $R_2$ are the gas constants for fuel mixture and combustion products respectively and $k_1$ is the adiabatic exponent for the fuel mixture.

The density ratio is given by one of the solutions of the resulting equation:

$$\frac{\bar{m}(1+k_{m2})}{2k_{m2}}\tau_r^2-(1+\bar{m})\tau_r+\frac{R_2}{R_1}+\frac{\bar{m}}{2k_{m2}}(k_{m2}-1)+\frac{\alpha(k_{m2}-1)}{k_{m2}}=0\ ;\quad \alpha=\frac{q}{R_1T_1} \tag{8a}$$

$$k_1 = \frac{\overline{c_p^{(1)}(\theta_1)}}{\overline{c_p^{(1)}(\theta_1)} - 1}; \quad k_{m2} = \frac{\overline{c_{pm}^{(1)}(\theta_1, \theta_2)}}{\overline{c_{pm}^{(1)}(\theta_1, \theta_2)} - 1} \tag{8b}$$

In the above relations, the dimensionless temperature θ and the dimensionless specific heat at constant pressure were introduced as follows:

$$\theta = \frac{T}{\Delta T_{\text{dim}}} \; ; \quad \overline{c_p(T)} = \frac{c_p(T)}{R} \tag{9}$$

$R$ being the gas constant and $\Delta T_{dim}$ an arbitrary temperature interval. For sake of simplicity, one takes $\Delta T_{dim}$ = 1000 K.

Since the equation (8a) has two solutions, two states are theoretically possible: a strong wave and a weak detonation wave. The most probable state, observed experimentally, corresponds however to the case when the two states coincide: this is the ***Chapman-Jouguet wave*** (CJ) characterized by the following parameters:

$$\tau_{rCJ} = \frac{k_{m2}(1 + \bar{m}_{CJ})}{(1 + k_{m2})\bar{m}_{CJ}}; \quad p_{rCJ} = \frac{1 + \bar{m}_{CJ}}{1 + k_{m2}}; \quad T_{rCJ} = \frac{R_1}{R_2} p_{rCJ} \tau_{rCJ} \tag{10}$$

The mass flow rate corresponding to a CJ wave is obtained by equating to zero the discriminant of the equation (8a). This condition leads again to an algebraic equation of second degree having the following solutions:

$$\frac{\bar{m}_{CJ}}{k_{m2}} = \sqrt{\delta + 1} \pm \sqrt{\delta} \; ; \quad \delta = \left[ k_{m2} \left( \frac{R_2}{R_1} - 1 \right) + \frac{R_2}{R_1} + \alpha \frac{k_{m2}^2 - 1}{k_{m2}} \right]^2 - 1 \tag{11}$$

The sign (+) in (11) corresponds to ***detonation wave*** ($M_1 > 1$) while the sign (–) corresponds to ***deflagration wave*** ($M_1 < 1$). By imposing $\overline{m}_{CJ} = k_1 M_1^2$ and taking the sign (+) in (11) one obtains the temperature after the detonation wave. The Mach number after the wave in either case is given by:

$$M_2 = \sqrt{\frac{k_{m2}}{k_2}} > 1 \; ; \quad M_{2e} = M_2 \sqrt{\frac{k_2}{k_{m2}}} = 1 \tag{12}$$

Then the state after the Chapman-Jouguet wave is critical in terms of an ***equivalent Mach number*** $M_{2e}$.

The values of the specific heats and enthalpies are calculated by using the NASA coefficients [6] arranged in a dimensionless form [7].

## 3. THE COMBUSTION OF $H_2$ IN AIR. THE FLOW PARAMETERS AFTER THE DETONATION WAVE

One considers the combustion of $H_2$ in air according to the following reaction:

$$H_2 + \frac{0.5}{0.2095}(1+\beta)\text{Air} = \\ = \text{H}_2\text{O} + \lambda_1\text{O}_2 + \lambda_2\text{N}_2 + \lambda_3\text{NO}_2 + \lambda_4\text{NO} + \frac{0.5}{0.2095}0.0096(1+\beta)\text{Ar} \tag{13}$$

For air one considers the mixture $(0.2095\,\text{O}_2 + 0.7809\,\text{N}_2 + 0.0096\,\text{Ar})$. A ratio $\beta$ of air excess is allowed as well as the formation of NO and $NO_2$. If one considers that all $O_2$ was consumed $(\lambda_1 = 0)$, the other coefficients are:

$$\lambda_2 = \frac{\lambda_3}{2} + \frac{0.5}{0.2095}\left(0.7809 + 0.5714\beta\right)\ ;\ \ \lambda_4 = \beta - 2\lambda_3;\ \ \lambda_3 \le \frac{\beta}{2} \tag{14}$$

Other dissociation reactions beside $NO_2$ are also possible (for example, $\text{H}_2\text{O} \rightarrow \text{OH} + 0.5\text{H}_2$), but we have considered NO formation to have an order of magnitude for a representative pollutant. The main factor is the temperature $T_2$ after the CJ wave, influencing the dissociation rate. Anyhow, the reaction of NO formation is energy consuming and this fact is clearly pointed out by our method of calculation. This is why, when no air excess is present $(\beta = 0)$, we can assume that no nitrogen oxide will form. Therefore, for $\beta = 0$, from (14) one obtains: $\lambda_2 = \frac{0.5}{0.2095}\cdot 0.7809$ ; $\lambda_3 = \lambda_4 = 0$. In a more general case, the coefficient $\lambda_3$ of $NO_2$ is taken as a parameter.

The flow parameters after the detonation wave are obtained by using the equations (10), (11) and (12), mainly the temperature $T_2$ and the dimensionless mass rate $\bar{m}_{CJ}$ giving the Mach number admitted before the wave. Some results of the calculation are given in Table 1.

*Table 1*

Flow parameters for a Chapman-Jouguet detonation wave

| $M_1$ | $\beta$ | $\lambda_{NO_2}$ | $\lambda_{NO}$ | $T_2$ [K] | $p_r$ | $\tau_r$ | $\bar{m}_{CJ}$ |
|---|---|---|---|---|---|---|---|
| 5.2066 | 0.400 | 0.100 | 0.200 | 2496.5 | 17.091 | 0.5781 | 38.136 |
| 5.0435 | 0.400 | 0.000 | 0.400 | 2319.8 | 16.099 | 0.579 | 35.866 |
| 4.4480 | 0.800 | 0.100 | 0.600 | 1807.3 | 12.564 | 0.585 | 27.896 |
| 4.3479 | 0.800 | 0.000 | 0.800 | 1712.9 | 11.980 | 0.588 | 26.655 |

## 4. THE STRUCTURE OF THE DETONATION WAVE

Once the global properties were determined, one can proceed to the study of the detonation wave structure. In principal, a detonation wave consists of two waves: a shock wave where the temperature of the gas mixture is increased, such that the combustion can take place, followed by a deflagration wave where the chemical reaction takes place. For analyzing the waves' structure, one needs the conservation laws in a differential form. One writes the conservation equations for steady viscous laminar flow in 1D. By adopting the usual notations $u$, $\rho$, $p$, $T$ for velocity, density, pressure and temperature, one has [1,2,3,9]:

$$\mathrm{d}(\rho u)=0\ ;\quad \rho u=\text{const.}\ ;\quad \rho_1 u_1=\rho_2 u_2\quad (\textit{continuity}) \tag{15}$$

$$\rho u\cdot \mathrm{d}u+\mathrm{d}\left(p-\frac{4}{3}\mu\frac{\mathrm{d}u}{\mathrm{d}x}\right)=0\quad (\textit{momentum}) \tag{16}$$

$$\rho u\cdot \mathrm{d}h^*=\mathrm{d}\left[\lambda_T\frac{\mathrm{d}T}{\mathrm{d}x}+\frac{4}{3}\mu\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{u^2}{2}\right)\right]=0\ ;\quad h^*=h+\frac{u^2}{2}\quad (\textit{energy}) \tag{17}$$

where $h$, $\lambda_T$, $\mu$ are the enthalpy, the thermal conductivity and the dynamic viscosity respectively, all of them depending on temperature. One considers laminar flow.

One starts with integrating once the energy equation (17), and writing it in a form containing the Prandtl number Pr and the total enthalpy $h^*$:

$$\rho u\left(h^*-h_1^*\right)=\frac{4}{3}\mu\frac{\mathrm{d}}{\mathrm{d}x}\left[h^*+\left(\frac{3}{4\,\mathrm{Pr}}-1\right)\frac{u^2}{2}\right]\ ;\qquad \mathrm{Pr}=\frac{\mu c_p}{\lambda} \tag{18}$$

The term containing the velocity $u$ is small in comparison with the total enthalpy; in addition, it has a small coefficient as the Pr number has values around 0.75 [2]. Then, one takes the simplified energy equation:

$$\rho u\left(h^*-h_1^*\right)=\frac{4}{3}\mu\frac{\mathrm{d}h^*}{\mathrm{d}x}\ . \tag{19}$$

having the solution $h^*=h_1^*=\text{const.}$ Therefore, the total enthalpy remains constant even inside the waves.

By integrating the momentum equation (16) once, one obtains:

$$\frac{4}{3}\mu\frac{\mathrm{d}u}{\mathrm{d}x}=p-p_1+\rho u^2-\rho_1 u_1^2;\quad p_1+\rho_1 u_1^2=p_2+\rho_2 u_2^2 \tag{20}$$

Since the derivatives with respect to $x$ are equal to zero before as well as after the wave, one re-finds the equation (2). The flow is considered laminar and for the viscosity $\mu$, the formula of Sutherland was used (see below).

For turbulent regimes the viscosity should be adapted [10].

**The structure of the shock wave**

One adopts the indexes "1" at entrance and "s" at wave exit. In order to obtain the pressure, density and the temperature at the shock exit, the algebraic form of conservation laws (15), (16), (17) is used. The already established relations (7), (8a), (8b) are used for $R_1 = R_2$, $q = 0$ to obtain:

$$\begin{aligned} &p_{rs} = (1+\chi_{ms})M_{1e}^2 - \chi_{ms}; \quad \rho_{rs} = \chi_{ms} + \frac{1-\chi_{ms}}{M_{1e}^2}; \\ &\theta_{rs} = p_{rs}\rho_{rs}; \quad \chi_{ms} = \frac{k_{ms}-1}{k_{ms}+1}; \quad M_{1e}^2 = \frac{k_1}{k_{ms}}M_1^2 \end{aligned} \tag{21}$$

$M_{1e}$ being the equivalent number in the shock transformation. Some values are given in Table 2.

*Table 2*

Flow parameters for the shock wave

| $M_1$ | $M_{1e}$ | $\theta_{rs}$ | $p_{rs}$ | $\tau_{rs}$ | $M_s$ | $\bar{m}_{CJs}$ | $z_s=1-u_{rs}$ |
|---|---|---|---|---|---|---|---|
| 5.2066 | 5.2851 | 5.9246 | 32.094 | 0.1846 | 0.4063 | 0.2195 | 0.8154 |
| 4.3479 | 4.4158 | 4.4372 | 22.367 | 0.1984 | 0.4179 | 0.2364 | 0.8016 |

To solve the equation (20), one introduces the ratio $u_r = u/u_1$ for velocities, the new variable $z$ and the law of Sutherland for the gas viscosity, as follows:

$$z = 1-u_r; \quad u_r = u/u_1; \quad \frac{\mu(\theta)}{\mu_1} = \theta^{\frac{1}{2}}\left(1+C_S/\theta_1\right)/\left(1+C_S/\theta\right) \tag{22}$$

$C_S$ being the Sutherland constant adapted for the dimensionless temperature $\theta_1$ ($C_S = 0.122$ for air). The equation (20) is integrated under the form:

$$\frac{3p_1}{4\mu_1 u_1}\left(x-x_1\right) = \int_{\varepsilon}^{z}\frac{\mathrm{d}z}{\Phi(z)}; \quad \Phi(z) = \frac{\mu_1}{\mu(\theta)}\left(1-\frac{\theta_r}{1-z}+\bar{m}z\right); \quad \bar{m} = k_1 M_1^2 \tag{23}$$

where the small number $\varepsilon > 0$ was introduced at the lower limit of the integral in order to avoid singularities.

The function $\Phi(z)$ has two zeros, at $z=0$ and $z=z_s=1-u_{rs}$ which are singularities for our equation. One can obtain an accurate analytical expression by using an interpolation polynomial passing through five points: $z_{k+1}=kz_s/4$ where $k=0,1,2,3,4$, in the form:

$$\Phi(z)\cong z(z_s-z)\left(az^2+bz+c\right);\quad \frac{1}{\Phi(z)}=\frac{A}{z}+\frac{B}{z_s-z}+\frac{A_1z+B_1}{az^2+bz+c} \tag{24}$$

The coefficients $A_1, B_1$ are depending on the sign of the discriminant $\Delta=b^2-4ac$. In this case, the second degree polynomial in (24) has complex conjugate roots. The solution is:

$$\frac{3p_1}{4\mu_1u_1}(x-x_1)=\int\frac{dz}{\Phi(z)}=\ln\left[\frac{z^A}{(z_s-z)^B}\right]+\frac{A_1}{2a}I_1(z)+\left(B_1-\frac{bA_1}{2a}\right)I_2(z) \tag{25a}$$

$$I_1(z)=\ln\left(az^2+bz+c\right);\quad I_2(z)=\frac{2}{\sqrt{-\Delta}}\arctan\left(\frac{2az+b}{\sqrt{-\Delta}}\right) \tag{25b}$$

being represented in Figs. 2 and 3.

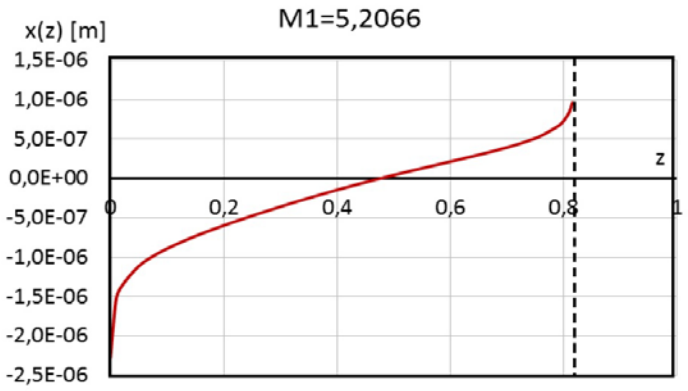


Fig. 2 – The shock wave structure for $M_1$ = 5.2066

In Fig. 2 and Fig. 3, the shock wave structure is represented by showing the displacement $x$ as a function of the velocity parameter $z$ for two values of inlet speed $M_1$. The thickness of shock wave is estimated to be of order of $3\cdot10^{-6}$ m and $4\cdot10^{-6}$ m, respectively (which is a quiet large value due to the small pressure at high altitude).

**The structure of the deflagration wave**

In order to obtain the values of the gas parameters inside the deflagration wave, one introduces a variable which describes the reaction advance from $q_s = 0$ after the shock wave to the completion of combustion.

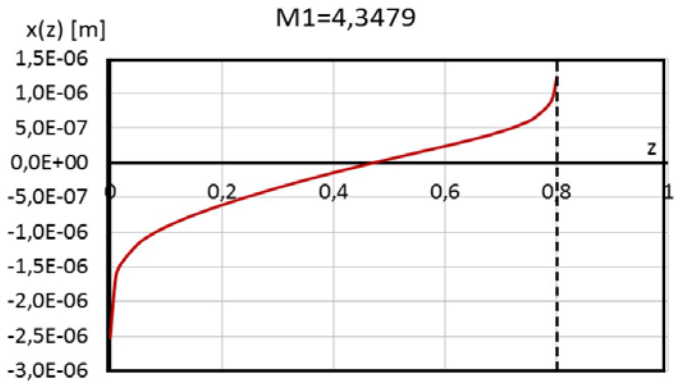


Fig. 3 – The shock wave structure for $M_1 = 4.3479$

Let $\gamma(z)$ be a parameter indicating the reaction evolution such that:

$$\sum(1) = \gamma\sum(2) + (1-\gamma)\sum(1)\,; \quad \sum(1) = \mathrm{H_2} + \frac{0.5}{0.2095}(1+\beta)\mathrm{Air} \tag{26a}$$

$$\sum(2) = \mathrm{H_2O} + \lambda_1\mathrm{O_2} + \lambda_2\mathrm{N_2} + \lambda_3\mathrm{NO_2} + \lambda_4\mathrm{NO} + \frac{0.5}{0.2095}0.0096(1+\beta)\mathrm{Ar} \tag{26b}$$

One takes:

$$\gamma(z) = \left(\frac{z}{z_5}\right)^{\omega}, \quad \omega \in (0;\,1)\,; \quad z = \frac{u}{u_s} - 1 \tag{26c}$$

The states described by the equations (26a,b,c) are computed for five values of $\gamma(z)$, the initial and the final ones being known. The differential equation to be solved for the deflagration wave structure is:

$$\frac{4}{3}\mu\frac{\mathrm{d}u}{\mathrm{d}x} = p + \rho u^2 - p_s - \rho_s u_s^2 \tag{27}$$

One problem is related to the viscosity values for various gas mixtures. One maintains the equation already used in case of the shock wave structure and adjusts the value of the Sutherland constant which becomes a function of $\gamma$: $C_s = C_s(\gamma)$.

A control of the values given to γ(z) is possible by observing that $\frac{\mathrm{d}u}{\mathrm{d}x} \geq 0$ for deflagration waves. The equation for $\gamma = 1.0$ was first solved for the whole detonation wave in order to obtain the mass rate parameter $\bar{m}$ and the Mach number at entrance $M_1$ permitted for the Chapman-Jouguet detonation wave (see Table 1). Then, by maintaining the obtained mass rate, the flow parameters have been calculated for the introduced reaction heat $q(\gamma)$, according to the reactions (26a), (26b) and starting from the shock wave. Since the Mach number after the shock wave is less than one, the process corresponds to a deflagration wave (the sign (–) in the equation (8a)). An interpolation polynomial was used like in the case of the shock wave.

The equation to be solved is:

$$\frac{3p_s}{4\mu_1 u_s}x = \int_{\varepsilon}^{z} \frac{\mathrm{d}z}{\Phi_s(z)}\ ;\quad \Phi_s(z) = \frac{\mu_1}{\mu(\theta)}\left(\frac{\theta_r}{1+z} - 1 + \bar{m}_s z\right)\ ;\quad \bar{m}_s = \frac{k_1 M_1^2 \tau_{rs}}{p_{rs}}\ ;$$
$$z = u_e - 1\ ;\quad \theta = \frac{R_1}{R_2} p_r \tau_r \tag{28}$$

The calculation is similar to the case of the shock wave structure; some results are presented in Fig. 4 for $\omega = 0$, Fig. 5 for $\omega = 0.2$ and Fig. 6 for $\omega = 0.24$.

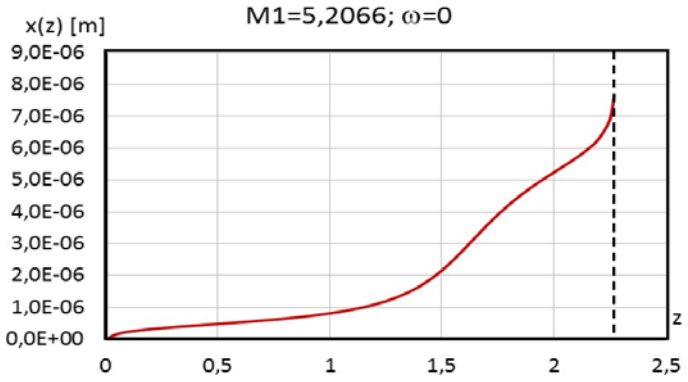


Fig. 4 – The velocity distribution inside the deflagration wave for $M_1 = 5.2066$ and $\omega = 0$

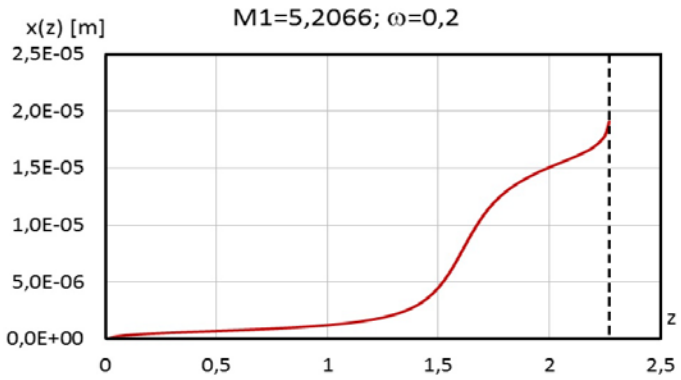


Fig. 5 – The velocity distribution inside the deflagration wave for $M_1$ = 5.2066 and ω = 0.2

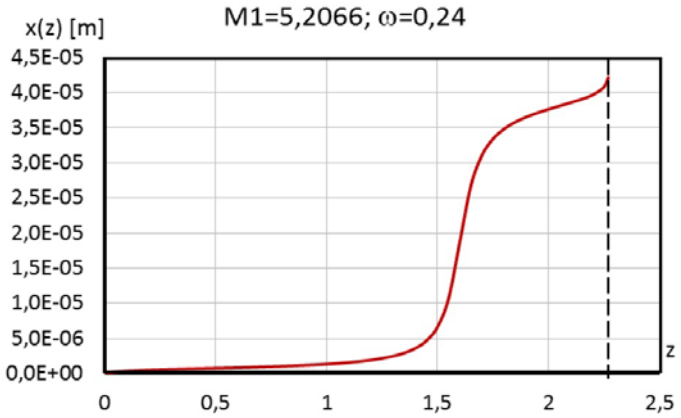


Fig.6 – The velocity distribution inside the deflagration wave for $M_1$ = 5.2066 and ω = 0.24

## 5. CONCLUSIONS

The structure of the detonation wave obtained for the combustion of $H_2$ in air in a hypersonic flow engine at high altitude was studied. To this aim the detonation wave as a whole was first calculated in order to determine the admitted Chapman-Jouguet mass flow rate and the possible Mach number before the detonation wave. This was made easier by the form of the energy equation with average specific heats given by one of the authors [7], which permits a direct analogy with the case of the constant specific heats. The temperature after the Chapman-Jouguet combustion was also calculated. Then, the less detailed structure of the detonation wave composed of a shock wave and a deflagration wave was considered. The shock wave is a normal one, the Mach number being less then unity after it. Therefore the combustion after the shock wave is subsonic, the gas being accelerated up to a critical state in terms of an equivalent Mach number

introduced in [7]. The detailed structure of the shock wave was described by solving the momentum differential equation in velocity and a distance through the wave. By taking four intervals within the wave and using an interpolation function, an analytical solution was obtained putting two logarithmic singularities in evidence. Figures for the velocity variation within the shock wave and values for temperatures inside the shock wave are given.

After the shock wave, the deflagration Chapman-Jouguet wave was studied. As a verification, the final temperature $T_2$ was re-found. In order to establish a parameter for the deflagration wave structure, the degree of the combustion advance in terms of the reaction was introduced, by correspondingly adapting the global chemical reaction without detailed chemical kinetics. The momentum differential equation in velocity and a distance through the wave thickness was solved again for more complicated functions for velocity, pressure and temperature. An analytical expression was obtained again with two logarithmic singularities at the wave ends. Three cases corresponding to different reaction speeds were considered, one of them leading to temperatures proper to dissociation although these temperatures are decreasing to the end of deflagration wave.

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