NUMERICAL SOLUTIONS FOR COMBUSTION WAVE VELOCITY

Constantin ROTARU

”Henri Coandă” Air Force Academy, Braşov, Romania (rotaru.constantin@afahc.ro)

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Abstract: *Starting from the basic equations of mass, momentum and energy, in this paper are presented some aspects regarding the gas-dynamic model of the detonation wave, where the combustion wave speed was obtained from a given initial conditions. The compatibility, the existence and the unicity of the solution with the dynamics of the combustion behind the wave depend on the singularities of dimensionless forms of momentum and species conservation equations. This combustion model can be extended to others propulsion systems which are designed for a high thrust and velocity.*

Keywords: *propulsion systems, combustion, shock waves, detonation, deflagration*

1. INTRODUCTION

In a combustion process can appear two types of self-propagating waves: deflagration which propagates at subsonic velocities and depend not only on the initial state of the combustion mixture but also, on the boundary conditions behind the waves and detonation which has a transient three-dimensional structure 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. Deflagration has a velocity, proportional to the square root of the reaction rate and in stationary conditions it is defined as a flame, while 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 deflagration and detonation can be distinguished from each other: by the expansion (deflagration) versus compression (detonation) nature of the wave; by their propagation speed; a deflagration wave propagates via the diffusion of heat and mass from the flame zone to effect ignition in the reactants ahead; deflagration requires fractions of the millijoule of energy for ignition, whereas a detonation requires joules (or kilojoules) for ignition; a detonation wave is a supersonic compression shock wave that ignites the mixture by heating across the leading shock front. The transition from deflagration to detonation in a long smooth tube, occurs when the velocity is about half the Chapman-Jouguet (CJ) detonation speed and from gas-dynamic considerations, deflagration solutions are represented on the lower branch of the Hugoniot curve and the maximum deflagration speed (for a given initial state ahead of the flame) corresponds to the point where the Rayleigh line and the Hugoniot curve are tangent, therefore, for detonations, the solution is represented on the upper branch of this curve and the minimum velocity detonation solution corresponds to the tangency of the Rayleigh line to the Hugoniot curve on the on the upper branch.

For a propagating deflagration wave, a precursor shock is usually generated ahead of the flame and this precursor shock changes the initial state ahead of the flame and depending on its strengths, will result different deflagration solutions.

The rate of mass burnt gas increase inside a spherical flame of radius *r* is $4\pi r^2 \rho_0 v_0$ and since the mass of burnt gas is $\frac{4}{3}\pi r^3 \rho_\infty$ it follows that the flame speed is $v_0 = \frac{\rho_\infty}{\rho_0}\frac{dr}{dt}$ and it depends on the pressure, temperature and composition of the initial combustible mixture, where ρ_0 is the density of the unburnt mixture and ρ_∞ is the density of burnt gas. The burning velocity v_0 can be related to the wave thickness δ considering a stationary plane deflagration with *q*-the heat of reaction, *w*-the reaction rate and $q \cdot \delta \cdot w$ the energy released per unit area of the wave, per second. For an adiabatic process no energy is lost from the sides of the wave, then $q = c_p\left(T_\infty - T_0\right)$, where c_p is the average specific heat of the mixture and T_∞ is the burnt gas temperature and the rate of which heat is conducted upstream is $\lambda dT/dx \cong \lambda\left(T_\infty - T_0\right)/\delta$, where *T* is the temperature, λ is the mean thermal conductivity of the gas and *x* is the distance normal to the wave. From the equation $c_p\left(T_\infty - T_0\right)w \cdot \delta = \lambda\left(T_\infty - T_0\right)/\delta$ it follows that $\delta = \sqrt{\lambda/\left(c_p \cdot w\right)}$, the combustible material mass flow rate following into the wave is $\rho_0 v_0$ and the deflagration wave consumes these reactants at the rate $w \cdot \delta$ (mass per unit area per second), therefore $\rho_0 \cdot v_0 = w \cdot \delta$ which yields to $v_0 = \sqrt{\lambda w / c_p} / \rho_0$. In these expressions, *w* is the factor with the strongest temperature dependence, which varies as $e^{-\frac{E}{R^0 T}}$, where *E* is the activation energy and R^0 is the universal gas constant.

2. COMBUSTION WAVES

Under some assumptions (one step first order reaction in a binary mixture with a Lewis number of unity and an effective Prandtl number of ¾; the effective coefficient of viscosity equals the ratio of the thermal conductivity to the average specific heat, λ / c_P; all chemical species may be considered to have constant and equal average specific heats at constant pressure, c_p), the structure of a combustion wave can be analyzed, based on the following system of equations

$$\begin{cases} \dfrac{d\varphi}{d\tau} = \dfrac{\varphi - 1 + \dfrac{1}{\gamma M_0^2}\left\{\dfrac{1}{\varphi}\left[1 + \alpha'\tau - \dfrac{\gamma - 1}{2} M_0^2\left(\varphi^2 - 1\right)\right] - 1\right\}}{\tau - \varepsilon} \\ \dfrac{d\varepsilon}{d\tau} = \dfrac{\dfrac{\lambda \rho B_1 T^{\alpha_1}}{m^2 c_p}\left(1 - \tau\right) e^{-\frac{E_1}{R^0 T}}}{\tau - \varepsilon} \end{cases} \tag{1}$$

where $\varphi = \frac{v}{v_0}$; ε is the reaction progress variable ; *q* – the total heat release per unit mass of mixture; q – the total heat release per unit mass of mixture;

M_0 is the Mach number, γ is the specific heats ratio; B_1 is a constant of reaction; T is the temperature; $\tau = \dfrac{\left(c_p T + \dfrac{v^2}{2}\right) - \left(c_p T_0 + \dfrac{v_0^2}{2}\right)}{q}$; $\alpha' = \dfrac{q}{c_p T_0}$; ε is the reaction progress variable.

These differential equations have the boundary conditions:

$$\text{at } \tau = 0 \quad \Rightarrow \quad \begin{cases} \varepsilon = 0 \\ \varphi = 1 \end{cases} \text{ and at } \tau = 1 \quad \Rightarrow \quad \begin{cases} \varepsilon = 1 \\ \varphi = \varphi_\infty \end{cases} \tag{2}$$

In the three dimensional $(\varepsilon, \varphi, \tau)$ space, the solutions of the system (1) are lines, beginning at the point $(0, 1, 0)$ and ending at the point $(1, \varphi_\infty, 1)$ and they must lie within a region of semi-infinite beam of unit square cross section (fig. 1), with the singularities of equations (1) located at the points where both the numerator and the denominator vanish. When $\varepsilon = \tau$ the denominators vanish (which defines a plane containing the φ axis), and the numerators of equations vanish when

$$\begin{cases} \varphi - 1 + \dfrac{1}{\gamma M_0^2}\left\{\dfrac{1}{\varphi}\left[1 + \alpha'\tau - \dfrac{\gamma - 1}{2} M_0^2\left(\varphi^2 - 1\right)\right] - 1\right\} = 0 \\ \dfrac{\lambda \rho B_1 T^{\alpha_1}}{m^2 c_p}(1 - \tau) e^{-\frac{E_1}{R^0 T}} = 0 \end{cases} \tag{3}$$

The solutions of the above equations define cylindrical surfaces with the generatrices parallel to the ε axis.

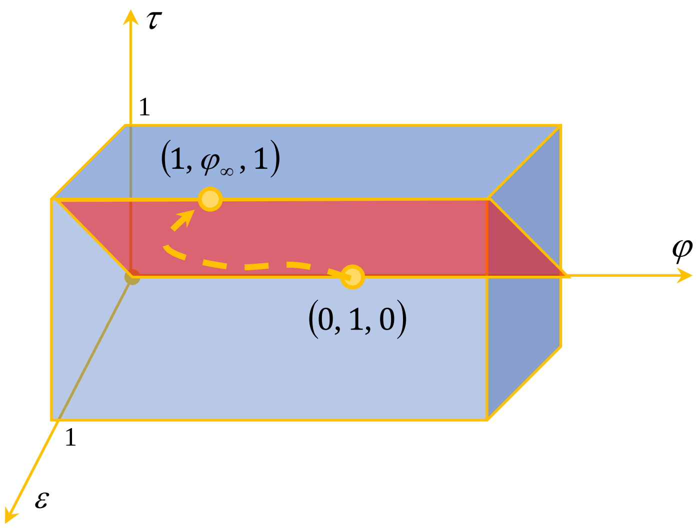


FIG.1 The boundary conditions for equations (1)

3. DETONATION WAVE STRUCTURE

For a perfect gas with a constant specific heat ratio, γ, the one-dimensional gas-dynamic equations are given as

$$\begin{cases} \dfrac{\partial\rho}{\partial t}+\rho\dfrac{\partial u}{\partial r}+u\dfrac{\partial\rho}{\partial r}+\dfrac{j\rho u}{r}=0 \\ \dfrac{\partial u}{\partial t}+u\dfrac{\partial u}{\partial r}+\dfrac{1}{\rho}\dfrac{\partial p}{\partial r}=0 \\ \left(\dfrac{\partial}{\partial t}+u\dfrac{\partial}{\partial r}\right)\dfrac{p}{\rho^{\gamma}}=0 \end{cases} \tag{4}$$

where *j* denotes the cylindrical ($j=1$), planar ($j=0$) and spherical symmetry ($j=2$). In the case of a steady detonation wave at constant velocity, *D*, the entropy increase is the same, being valid the following isentropic relationship:

$$\frac{T}{p^{\frac{\gamma-1}{\gamma}}}=const.; \quad \frac{T}{\rho^{\gamma-1}}=const. \tag{5}$$

The temperature T can be replaced, starting from the sound speed expression, $c^2=\gamma RT$, with the sound speed,

$$\frac{c}{p^{\frac{\gamma-1}{2\gamma}}}=const.; \quad \frac{c}{\rho^{\frac{\gamma-1}{2}}}=const. \tag{6}$$

Replacing the pressure *p* and the density ρ, by the sound speed *c* and the velocity *u* (which are the dependent variable), equations (1) can be written as

$$\begin{cases} \dfrac{\partial c}{\partial t}+c\dfrac{\gamma-1}{2}\dfrac{\partial u}{\partial r}+u\dfrac{\partial c}{\partial r}+\dfrac{\gamma-1}{2}\dfrac{jcu}{r}=0 \\ \dfrac{\partial u}{\partial t}+u\dfrac{\partial u}{\partial r}+c\dfrac{2}{\gamma-1}\dfrac{\partial c}{\partial r}=0 \end{cases} \tag{7}$$

With the following nondimensional transformation of dependent and independent variables, simple progressive wave solution for the flow behind the detonation can be obtained

$$\begin{cases} \varphi(\xi)=\dfrac{u}{D} \\ \eta(\xi)=\dfrac{c}{D} \end{cases} \tag{8}$$

where $\xi=\dfrac{r}{D\cdot t}$.

Replacing the derivatives for c and u in the equations (7) we can obtain the expressions for $\varphi'(\xi)$ and $\eta'(\xi)$,

$$\begin{cases} \varphi'(\xi) = \dfrac{j\varphi(\xi)}{\xi}\dfrac{\eta^2(\xi)}{[\varphi(\xi)-\xi]^2-\eta^2(\xi)} \\ \eta'(\xi) = -\dfrac{\gamma-1}{2}\dfrac{j\eta(\xi)\varphi(\xi)}{\xi}\dfrac{\varphi(\xi)-\xi}{[\varphi(\xi)-\xi]^2-\eta^2(\xi)} \end{cases} \tag{9}$$

For the planar case we get the trivial solutions, $\varphi'(\xi)=0$ and $\eta'(\xi)=0$, or else $\varphi'(\xi)$ and $\eta'(\xi)$ are nonzero but the denominator of the above equations is zero, $[\varphi(\xi)-\xi]^2-\eta^2(\xi)=0$. The solutions $\varphi(\xi)=0$ and $\eta(\xi)=0$, correspond to an uniform flow behind the planar detonation and from equation $[\varphi(\xi)-\xi]^2-\eta^2(\xi)=0$, it follows that

$$\begin{cases} \varphi(\xi) = \dfrac{2}{\gamma+1}(\xi-1)+\varphi_1 \\ \eta(\xi) = \dfrac{\gamma-1}{\gamma+1}(\xi-1)+\eta_1 \end{cases} \tag{10}$$

where φ_1 and η_1 are the constants, evaluated from the boundary conditions (the front, $\xi=1$). The particle velocity decreases to zero at about half the distance that the detonation has propagated from the closed end of the tube, because the value of ξ for which $\varphi(\xi)=0$ is $\xi=1-\dfrac{\gamma+1}{2}\varphi_1$ and for a strong detonation, where the particle velocity can be approximated by $\varphi_1=\dfrac{1}{\gamma+1}$ it follows that $\xi=0.5$, therefore, the Chapman-Jouguet condition at the detonation front gives $\varphi|_{\xi=1}+\eta|_{\xi=1}=1$, and $u|_{\xi=1}+c|_{\xi=1}=D$.

In the stagnant region of the detonation product, the pressure can be calculated as

$$\frac{p}{p_1} = \left(\frac{\eta|_{\varphi=0}}{\eta_1}\right)^{\frac{2\gamma}{\gamma-1}} \tag{11}$$

and for the regions where $\xi=0.5$ and $\xi=1$, it follows that

$$\frac{p|_{\xi=0.5}}{p|_{\xi=1}} == \left(\frac{\frac{1}{2}}{\frac{\gamma}{\gamma+1}}\right)^{\frac{2\gamma}{\gamma-1}} \tag{12}$$

This ratio becomes $p\big|_{\xi=0.5} / p\big|_{\xi=1} = 0.34$, for the case when $\gamma = 1.4$ and at the open end of the tube, where $x = 0$ (and $\xi = 0$), the flow reverses and propagates away from the detonation, toward the tube exit, and the velocity can be obtained from the equations (10), $\varphi(0) = -1/(\gamma+1)$ and $\eta(0) = 1/(\gamma+1)$that means the pressure at the open end is

$$\frac{p\big|_{\xi=0}}{p\big|_{\xi=1}} == \left(\frac{\frac{1}{\gamma+1}}{\frac{\gamma}{\gamma+1}}\right)^{\frac{2\gamma}{\gamma-1}} = 0.1 \tag{13}$$

The detonation velocity is linear dependent on the tube diameter (fig. 2), and it permits an interpolation of the straight line to infinite tube diameter, in order to get a value of the detonation velocity, D_∞, which can be considered independent of the tube diameter. The behavior of the detonation velocity for the large-diameter tubes, may not follow the inverse tube diameter dependence, when the boundary layer thickness become negligible compared to the tube diameter and the flow in the reaction zone can be approximated as quasi-one-dimensional. The Mach number at the CJ plane is equal to unity, an expression for M_1 is given by

$$M_1 = \left[\frac{Q}{c_1^2}(\gamma_1 - 1) - \frac{\gamma_1 - \gamma_2}{\gamma_1(\gamma_2 - 1)}\right]\sqrt{\left(\frac{\gamma_2^2 - 1}{\gamma_1 - 1}\right)\frac{1}{1+\gamma_2^2\psi}} \tag{14}$$

where

$$\psi = \left(\frac{1}{1-\nu}\right)^2 - 1;\ \nu = \frac{\varepsilon\xi}{(\gamma_2+1)(1+\xi)};\ \ \xi = \frac{A_2}{A_1} - 1 \tag{15}$$

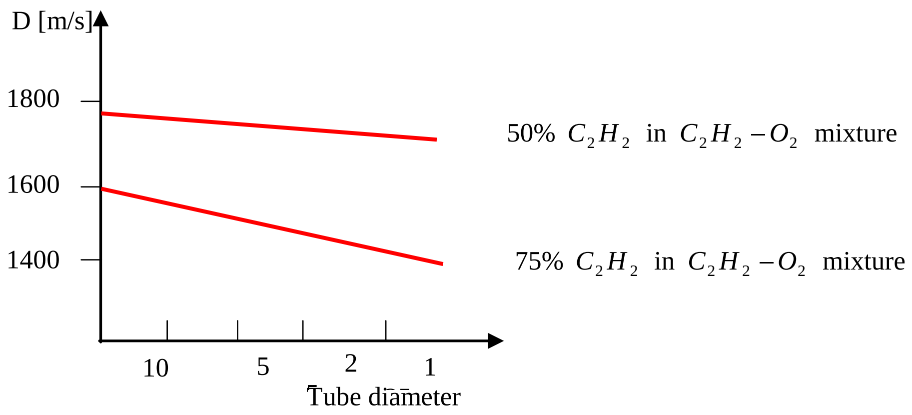


FIG. 2 The dependency of the detonation velocity on the tube diameter

The velocity deficit may be written as a function of the thickness, δ^*, of the boundary layer, where $\xi = 4\delta^*/d$, in the followings form

$$\frac{\Delta V_1}{V_1} = \frac{4\gamma_2^2}{\gamma_2 + 1} \frac{\delta^*}{d} \tag{16}$$

It was found, experimentally that the reaction zone thickness is a function of the detonation velocity and the critical tube diameter, d_c (which represents the minimum diameter through which a planar detonation can be developed in a spherical detonation), therefore, the detonation induction distance (the distance travelled by the flame before detonation onset) can be increased by more three times when the wall of the detonation tube is lined with an acoustically attenuating material such as porous sintered bronze. For high pressure behind the wave front, the ratio of densities approaches a certain finite value, being equal to

$$\frac{\rho_1}{\rho_0} = \frac{\gamma + 1}{\gamma - 1} \tag{17}$$

which leads to the following limiting values: for monoatomic gas with $\gamma = 5/3$ the density ratio is equal to 4, for diatomic gas with $\gamma = 7/5$, it is equal to 6 and for the full vibrational excitation case, $\gamma = 9/7$ and the density ratio is equal to 8. The density increases very slowly at high pressure p_1,. in the limit of a strong shock, the following expressions being valid

$$\frac{T_1}{T_0} = \frac{\gamma - 1}{\gamma + 1} \frac{p_1}{p_0}; \quad u_0 = \sqrt{\frac{\gamma + 1}{2} \frac{p_1}{\rho_0}}; \quad u_1 = \sqrt{\frac{(\gamma - 1)^2}{2(\gamma + 1)} \frac{p_1}{\rho_0}} \tag{18}$$

With respect to the discontinuity, the gas velocities divided by the speed of sound are given by

$$\left(\frac{u_0}{c_0}\right)^2 = \frac{(\gamma - 1) + (\gamma + 1)\frac{p_1}{p_0}}{2\gamma}; \quad \left(\frac{u_1}{c_1}\right)^2 = \frac{(\gamma - 1) + (\gamma + 1)\frac{p_0}{p_1}}{2\gamma} \tag{19}$$

For the weak shock wave $p_1 \approx p_0$ and $\rho_1 \approx \rho_0$, (the pressures on both sides of the discontinuity are close to each other), therefore the sound speeds are almost equal, $c_1 \approx c_0$, that means, a weak shock wave travels through the gas with a velocity which is very close to the speed of sound, while for a shock wave, across which the gas is compressed $(\rho_0 < \rho_1)$ and $(p_1 > p_0)$ the gas flows into the discontinuity with a supersonic velocity $(u_0 > c_0)$ and it flows out with a subsonic velocity $(u_1 < c_1)$In terms of the viscosity and thermal conductivity coefficients, the gas-dynamic equations are

$$\begin{cases} \rho u = \rho_0 u_0 \\ p + \rho u^2 - \dfrac{4}{3}\mu \dfrac{du}{dx} = p_0 + \rho_0 u_0^2 \\ \rho u\left(h + \dfrac{u^2}{2}\right) - \dfrac{4}{3}\mu u \dfrac{du}{dx} - k\dfrac{dT}{dx} = \rho_0 u_0 \left(h_0 + \dfrac{u_0^2}{2}\right) \end{cases} \tag{20}$$

where the constants of integration are considered as functions of the x coordinate, expressed in terms of the initial values of the variables p, ρ, T and velocity u, so, in order to describe the adiabatic motion of a fluid it is necessary to specify either the entropy or the specific internal energy as a function of density and pressure.

The presence of dissipative processes such as viscosity and heat conduction indicate the irreversibility of a shock compression, which lead to the increase in the entropy, so, the time it takes the fluid in a shock wave to go from the initial to the final state is very short, much shorter than the characteristic times over which the flow variables change in the continuous flow region behind the shock front. The front thickness is much less than the characteristic length scale over which the state of the gas behind the front changes significantly, therefore, the kinetics of the internal processes which take place within a shock front propagating through a gas with given initial conditions depend only on the wave strength. In a coordinate system moving with the wave front the one-dimensional flow equations for viscous and heat conducting gas flow, are

$$\begin{cases} \dfrac{d}{dx}\rho u = 0 \\ \rho u \dfrac{du}{dx} + \dfrac{dp}{dx} - \dfrac{d}{dx}\dfrac{4}{3}\mu \dfrac{du}{dx} = 0 \\ \rho u T \dfrac{d\sum}{dx} = \dfrac{4}{3}\mu\left(\dfrac{du}{dx}\right)^2 - \dfrac{dS}{dx} \end{cases} \tag{21}$$

where μ is the coefficient of viscosity, k represents the coefficient of thermal conductivity, $\sum$ is the specific entropy and S is a nonhydrodynamic energy flux, $S = -k\dfrac{dT}{dx}$. The constants of integration are expressed in terms of the initial values of the flow variables, distinguished by the subscript "0" and by the front velocity $D = u_0$. The dimensionless velocity $\eta = u / D = \rho_0 / \rho$ satisfies the equations

$$\frac{1-\eta(x)}{[\eta(x)-\eta_1]^{\eta_1}} = \frac{1-\sqrt{\eta_1}}{\left[\sqrt{\eta_1}-\eta_1\right]^{\eta_1}} \exp\left(1.1\frac{M^2-1}{M}\cdot\frac{x}{l_0}\right) \tag{22}$$

where η_1 refers to the final state behind the shock front

$$\eta_1 = \frac{\gamma-1}{\gamma+1} + \frac{2}{\gamma+1}\frac{1}{M^2} \tag{23}$$

and M is the Mach number, $M = D / c_0$ and c_0 is the speed of sound in the initial state.

The contribution of each of these coefficients to the formation of a shock are not equal, despite the fact that the values of the transport coefficients for kinematic viscosity and thermal diffusivity are close to each other. The equations for one-dimensional steady flow (by neglecting viscosity) take the form

$$\begin{cases} \rho u = \rho_0 u_0 \\ p + \rho u^2 = p_0 + \rho_0 u_0^2 \\ h + \dfrac{u^2}{2} + \dfrac{S}{\rho_0 D} = h_0 + \dfrac{D^2}{2} \end{cases} \tag{24}$$

In the absence of viscosity, it follows that in the process of shock compression, the state of a gas particle changes along a straight line in the pressure-density diagram

$$p = p_0 + \rho_0 D^2 (1-\eta) \tag{25}$$

The ratio of temperatures, T/T_0 and the energy flux, S can be calculated starting from the expression of the enthalpy, $h = \dfrac{\gamma}{\gamma-1}\dfrac{p}{\rho}$, as it follows

$$\frac{T}{T_0} = 1 + \gamma M^2 (1-\eta)\left(\eta - \frac{1}{\gamma M^2}\right) \tag{26}$$

$$S = -\frac{\rho_0 D^3}{2}\frac{\gamma+1}{\gamma-1}(1-\eta)(\eta-\eta_1) \tag{27}$$

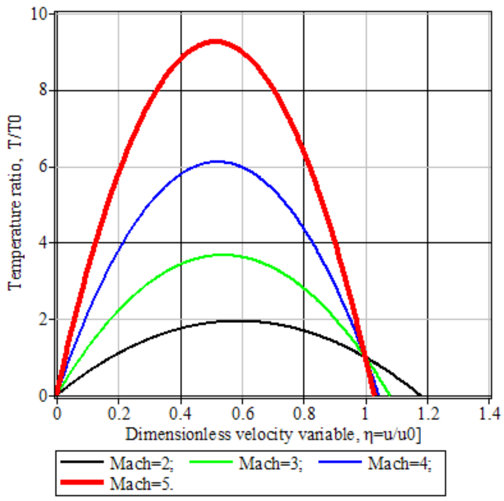
Here the dimensionless velocity in the final state, η_1 has the expression

$$\eta_1 = \frac{\gamma-1}{\gamma+1} + \frac{2}{\gamma+1}\frac{1}{M^2} \tag{28}$$

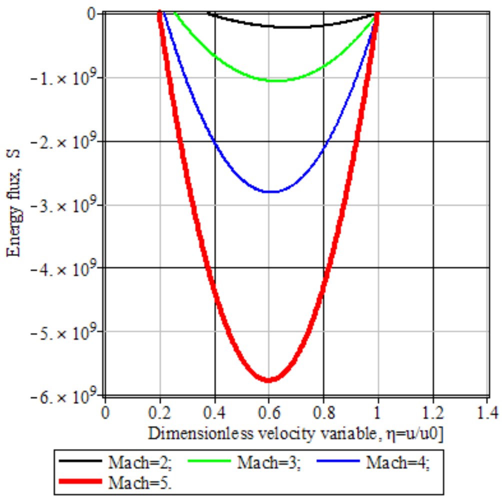
In Fig. 3 are resented the T/T_0 and S diagrams for the case of heat conduction.

The temperatures ratio has a maximum at the point $\eta = \dfrac{1}{2} + \dfrac{1}{2\gamma M^2}$, and if the shock is sufficiently weak, then η_1 is greater than this value. A monotonic increase in the temperature from the initial value T_0 to the final value T_1 (for a monotonic compression of the gas from the initial to the final volume) results and has the expression

$$\frac{T_1}{T_0} = 1 + \frac{2\gamma(\gamma-1)}{(\gamma+1)^2}(M^2-1)\left(1 + \frac{1}{\gamma M^2}\right) \tag{29}$$



(a)



(b)

FIG. 3. Temperature ratio (a) and energy flux (b)

CONCLUSIONS

The detonation velocity is independent of initial and boundary conditions but, due to the thickness of the reaction zone, the initial and boundary conditions can have a strong influence on the propagation of the detonation wave and on the instability of the detonation front, the effect of the boundary consisting in a velocity propagation reduction, a generating of traverse waves which have various positive and negative roles. The detonation velocity depends almost linearly on the inverse tube diameter and flames propagating upward, downward and horizontally in combustion chambers behave differently due to the buoyant effects. Combustion chamber walls have a great influence upon the flame motion and approximate values of flame speeds can be obtained by monitoring the pressure histories with data reduction performed on the basis of an assumed flame spherical shape with negligible thickness.

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