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Analysing some solid rocket double-base propellant ignition cases using the thermal theory

Dragan Lemić, PhD (Eng)¹⁾

The thermal theory of solid rocket propellant ignition based on the exothermic chemical reaction in the solid phase subsurface layer was analysed. Time-dependent equations controlling the process (the conservation of energy and components) were numerically solved, aiming at defining the temperature and concentration distribution in the solid phase. The calculated values of the characteristic parameters are in reasonable agreement with a large amount of experimental data from the references. Although the influence of the gas-phase reactions during the double-base rocket propellant ignition is obvious, the prospects of using the ignition theory while investigating the DB propellant ignition under certain conditions was demonstrated.

Key words: solid rocket propellant, double-base propellant, ignition, combustion.

Introduction

GENERALLY speaking, the solid rocket propellant ignition process consists of the inert heating (phase) and the chemical reactions phase. These reactions can occur in the solid phase, the gas-phase or between the two. Many investigations pointed out the important role of the gas phase reactions during the double-based propellants ignition process [1,4]. However, there are examples of a good correlation of the experimental data using the solid phase ignition theory [1,6]. The thermal or solid-phase ignition theory is the earliest of solid rocket propellant ignition theories. This theory is based on the assumption that the ignition process is controlled by the solid-phase conditions with temperature rise due to the heat transfer from an external thermal source and where the subsurface chemical reaction occurs. The mathematical formulation is simplified because the governing equations of the gas-phase processes are not included. Since only one part of the process is analysed, the ambient influence is not taken into account. However, under the conditions of lower external heat flux, high oxidizer concentration in the ambient gas and higher pressure, the solid propellant inert heating time is much longer than the time of diffusion or chemical reaction, so that the ignition delay can be close to the experimental results.

Application of the thermal theory in the investigation of double-base rocket propellants ignition

According to the thermal theory, the ignition of solid rocket propellants heated by an external source is initiated by exothermic chemical reactions of degradation occurring in the solid phase. A solid rocket propellant is treated as a semi-infinite plate with externally applied heat flux, to which the following expression for temperature variation

obtained from the unsteady energy conservation equation in the solid-phase, apply

$$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial x^2} + \frac{Q \cdot Z}{\rho c} \cdot \exp(-E/RT) \quad (1)$$

with the boundary and initial conditions

$$\begin{aligned} -\lambda \frac{\partial T}{\partial x} = \dot{q} \quad \text{at} \quad x = 0, t > 0 \\ -\lambda \frac{\partial T}{\partial x} = 0 \quad \text{for} \quad x \rightarrow \infty, t > 0 \end{aligned} \quad (2)$$

$$T = T_o \quad \text{for} \quad x \in \mathbb{R}, t = 0 \quad (3)$$

where Q [J/kg] is the thermal effect of the solid-phase exothermic chemical reaction, Z [1/s] pre-exponential factor in the law of the propellant mass decomposition rate $\omega = \rho Y Z \cdot \exp(-E/RT)$ and Y is the mass fraction of a non-reacted propellant. The solid propellant decomposition is defined by the initial component (solid propellant) mass conservation equation

$$-\frac{\partial Y}{\partial t} = Y Z \cdot \exp(-E/RT) \quad (4)$$

with the initial condition

$$Y_o = 1 \quad \text{for} \quad t = 0 \quad (5)$$

In the initial phase, due to the low propellant temperature, the heat produced by the chemical reaction is low, too. This is why the process can be divided into two phases. In the first phase („inert heating of propellant”) the heat conduction produced by the external source of energy is domi-

¹⁾ Military Technical Institute of the Yugoslav Army, Katanićeva 15, 11000 Beograd

nant. Due to this, the second term of the right side of eq.(4) can be omitted and the temperature distribution defined as in case of the nonreactive materials heating. The propellant temperature rise increases the importance and the contribution of the exotherm reaction heating in a solid rocket propellant layer near the surface. That is why the ignition delay time can be expressed as

$$t_{ig} = t_i + t_{ch} \tag{6}$$

where t_i is the propellant inert heating time with the external source and t_{ch} is the effective time of one exotherm reaction up to the self-sustained combustion.

Concerning the thermal theory, there are different criteria for defining the whole process of ignition or particular phases, given in references [1,3,4]. The critical temperature or gradient achieving is often used along with the production of a certain quantity of thermal energy in a heated propellant layer. A satisfactory correlation of a great number of experimental results published by different authors was obtained in reference [6] presuming that the thermal effect of the exotherm chemical reaction becomes, at one point, a significant part of the externally applied heat by conduction. The initial relation $\rho c(\partial T/\partial t) \approx \lambda(\partial^2 T/\partial x^2)$ of this process can be rewritten as

$$\int_0^\infty \rho Q Z \exp(aE/RT) dx = \phi \int_0^\infty \rho c \partial T/\partial t dx \tag{7}$$

or

$$\int_0^{x_r} \rho Q Z \cdot \exp(aE/RT) dx = \phi \int_0^{x_r} \rho c \partial T/\partial t dx \tag{8}$$

because the main part of the ignition process is confined to the surface layer with the depth x_r and in the time interval $Y \approx 1$. For an experimental definition of the ignition conditions, a constant value (i.e. transformed to $\dot{q} = \text{const.}$) of the externally applied heat flux is mainly used, so it is possible to apply the well-known dependence for a temperature profile in a nonreactive body in the first phase [8]

$$T(a,t) = (b - T_o) \sqrt{\pi} \operatorname{erfc} \frac{E}{2\sqrt{at}} \tag{9}$$

or

$$T(a,t) = T_o + (b - T_o) \sqrt{\pi} \cdot \frac{\operatorname{Erfi} \frac{E}{2\sqrt{at}}}{\sqrt{\pi}} \exp\left(-\frac{E^2}{4at}\right) \cdot \left[1 - \operatorname{erfc} \frac{E}{2\sqrt{at}}\right] \tag{10}$$

where $\operatorname{erfc} \frac{E}{2\sqrt{at}} = \frac{2}{\sqrt{\pi}} \int_0^y \exp(-\xi^2) d\xi$. Since the parameter

$\frac{b - T_o}{2\sqrt{at}} \frac{E}{\sqrt{\pi}}$ is significantly less than 1, it is possible to simplify the preceding equation and to obtain the following relation for the temperature field in the propellant heated layer

$$T(a,t) = T_o + (b - T_o) \sqrt{\pi} \operatorname{Erfi} \frac{E}{2\sqrt{at}} \tag{11}$$

Introducing this dependence into the left side of eq.(8) leads to

$$\int_0^{x_r} \rho Q Z \exp(bE/RT) dx = \int_0^{x_r} \rho Q Z \cdot \exp\left[\frac{E}{(b - T_o) \sqrt{\pi}} \operatorname{Erfi} \frac{E}{2\sqrt{at}}\right] dx \tag{12}$$

There is a relation between the surface temperature and the heat flux

$$T_s = T_o + \dot{q}_{ig} \frac{2}{\lambda} \cdot \sqrt{\frac{at}{\pi}} \tag{13}$$

so that

$$\int_0^{x_r} \rho Q Z \exp(bE/RT) dx = \int_0^{x_r} \rho Q Z \exp\left[\frac{E}{(b - T_o) \sqrt{\pi}} \operatorname{Erfi} \frac{E}{2\sqrt{at}}\right] \cdot \frac{\dot{q}_{ig}}{\lambda T_s} \cdot x_r dx \tag{14}$$

After integrating the final form of the left side of eq.(8), we obtain

$$\int_0^{x_r} \rho Q Z \exp(bE/RT) dx = \rho Q Z \exp\left[\frac{E}{(b - T_o) \sqrt{\pi}} \operatorname{Erfi} \frac{E}{2\sqrt{at}}\right] \cdot \frac{\lambda}{\dot{q}_{ig}} \cdot \frac{E}{RT_s} \cdot \frac{\dot{q}_{ig}}{\lambda T_s} \cdot x_r \tag{15}$$

Here $\beta_s = RT_s / E$. The right side of eq.(8) can be given as

$$\phi \int_0^{x_r} \rho c \frac{\partial T}{\partial t} dx \approx \phi \rho c \frac{E}{E} \frac{T_s}{T_s} \cdot x_r \tag{16}$$

From eq.(13), this relation follows

$$\frac{\partial T_s}{\partial t} = \frac{2\dot{q}_{ig}^2}{\lambda^2 (b - T_o) \sqrt{\pi}} \cdot \frac{a}{\pi} \tag{17}$$

The depth of the chemical reaction can be obtained from the mass reaction rate $\omega = \rho T Z \exp(aE/RT)$ reduction to a certain level, e.g. 10 % of its value at the propellant surface. This leads to

$$\frac{\exp[-E/RT(a,t)]}{\exp[-E/RT_s]} = \frac{1}{10} \tag{18}$$

so that the depth of the reaction in the solid rocket propellant is

$$x_r = \frac{\lambda \beta_s T_s}{\dot{q}_{ig}} \ln 10 \tag{19}$$

Along with eq.(17) it gives the following form to eq.(16)

$$\phi \int_0^{x_r} \rho c \frac{\partial T}{\partial t} dx \approx \phi \frac{\beta_s \dot{q}_{ig}}{T_s - T_o} \cdot \frac{\ln 10}{\pi} \tag{20}$$

Due to eqs.(15), (19) and (20) we can calculate the ignition temperature at the solid rocket propellant surface in the moment of the ignition criterion realization according to (7), from the following relation

$$\frac{9}{10} \rho Q Z \exp \left(\frac{E}{RT_s} \right) \frac{RT_s^2}{E} \cdot \frac{2 \dot{q}_{ig}}{T_s - T_o} \cdot \frac{RT_s^2}{E} \cdot \frac{\ln 10}{\pi} \quad (21)$$

The temperature of ignition is defined by the implicit dependence we get from eq.(21)

$$T_{s,ig} = \frac{E}{R \ln \left[\frac{\rho Q Z \lambda}{2 \dot{q}_{ig}} \exp \left(\frac{E}{RT_{s,ig}} \right) \frac{RT_{s,ig}^2}{E} - T_p \right]} \quad (22)$$

In reference [6] the authors got a good correlation of the experimental data for $\phi' = 0.15$. After the iterative computation of $T_{s,ig}$, the ignition delay time can be defined from eq.(19).

The model of adiabatic ignition developed by V.N.Viljunov [3,5] for a body with moderately increasing surface temperature (e.g. when heat is transferred from an external thermal source of constant intensity) belongs to the thermal theories group. The ignition period was also divided into the inert heating phase and the adiabatic phase of chemical reaction in a narrow zone near the propellant surface. In the first phase, the second term on the right side of eq.(1) is not taken into account. When the permanently increasing propellant surface temperature reaches some defined (characteristic) value, the exotherm chemical reaction with thermal effect considerably exceeding the heat quantity externally transferred to the propellant begins. For propellant temperature change in this phase the following relation is used

$$\frac{\partial T}{\partial t} \approx \frac{QZ}{c} \exp \left(\frac{E}{RT} \right) \quad (23)$$

The continuity of solutions for both phases results in the following expression

$$\frac{\pi}{2} \frac{\dot{q} \exp \left(\frac{E}{RT_*} \right)}{QZ \rho \lambda} \quad (24)$$

By introducing the effective width of the heated zone $x_* = \frac{\pi}{2} \frac{T_* - T_o}{\dot{q}}$ the author got

$$QZ \rho \exp \left(\frac{E}{RT_*} \right) \frac{\pi}{2} \cdot \frac{\lambda (T_* - T_p)}{\dot{q}} \quad (25)$$

treated as the steady equality of the heat generation rate in the volume ρx_* with a unit cross-section area, and the heat conduction into the cold propellant depth.

Eq.(25) can be transformed into

$$T_* = \frac{E}{R \ln \left[\frac{QZ \pi \rho \lambda (T_* - T_p)}{2 \dot{q}^2} \right]} \quad (26)$$

which is suitable for determining the temperature of chemical reactions initiation. From this condition, the expression for the ignition time is obtained

$$t_{ig} \approx \frac{1}{N} \frac{E (T_* - T_o)}{2 RT_*^2} \frac{RT_*^2}{Q} \cdot \frac{c}{QZ} \cdot \exp \left(\frac{E}{RT_*} \right) \quad (27)$$

Furthermore, the extrapolated ignition temperature is the temperature which, introduced into the solution of an inert body heat conduction equation, gives the total ignition time and is approximately

$$T_{ig} \approx T_* \left[1 + \frac{RT_*}{E} \frac{RT_*^2}{2E(T_* - T_o)} \right] \quad (28)$$

For the propellant *N* with 1%C added and the thermo-physical parameters $E = 1.4654 \cdot 10^3$ [J/mol], $Q = 1.13 \cdot 18^6$ [J/kg], $Z = 9.08 \cdot 10^{13}$ [s⁻¹], $\rho = 1600$ [kg/m³], $c = 1465$ [J/kgK], $\lambda = 0.2345$ [W/mK] ([5,7]) the difference between the ignition temperature and the temperature T_* at which chemical reactions become important, is about 3%. With higher values of external heat flux, this method gives higher ignition temperatures.

In reference [7], the nondimensional conservation equations of energy and concentration for reactive materials, were subjected to the Laplace transform. A direct connection between the parameters representing the solid propellant surface temperature and the concentration was established and an expression for nondimensional temperature change obtained. The expression was solved by the asymptotic expansion method, for $\Omega_0 = E(T_* - T_o) \gg 1$. In this way, the expression of chemical reactions occurrence time is determined

$$t_i = \frac{\pi}{4} \cdot \lambda \rho c \cdot \frac{(T_* - T_o)}{\dot{q}_{ig}^2} \quad (29)$$

The ignition time is

$$t_{ig} = \frac{\pi \lambda \rho c}{4} \cdot \frac{(T_* - T_o)}{\dot{q}_{ig}^2} \frac{RT_*^2}{E(T_* - T_o)} \cdot 2 \ln 2 \quad (30)$$

$$= t_i \frac{RT_*^2 \cdot 2 \ln 2}{E(T_* - T_o)}$$

and the implicit equation for the temperature of the body surface in the moment of ignition during the inert heating (extrapolated ignition temperature)

$$T_* = \frac{E}{R \ln \left[\pi Q Z \rho^m Y_o^m \lambda (T_* - T_o) \frac{c}{2 \dot{q}^2} \right]} \quad (31)$$

For the chemical reaction of the first order ($m=1$) and the initial concentration of the reactive matter $Y_o = 1$, the obtained relation is equal to that expressed by eq.(26). Furthermore, the relation (29) corresponds to the dependence (13) for heating an inert body by the constant intensity flux.

From eq.(30) a relatively small difference between the solid propellant ignition time and the beginning of the chemical reactions effect can be seen. The difference at $T = 20^\circ\text{C}$ is about 10% for the Russian propellant *N* with 1%C added [5,7] and 8% for the French propellant [6] ($E = 1.6747 \cdot 10^5$ [J/mol], $Q = 2.512 \cdot 10^5$ [J/kg], $Z = 1 \cdot 10^{-17}$ [s⁻¹], $\rho = 1600$ [kg/m³], $c = 1674.72$ (J/kgK), $\lambda = 0.2135$ [W/m²K]).

Table 1

\dot{q}_{ig} [MW/m ²]		0.01256	0.041868	0.18422	0.41868	0.45636	0.8918	4.1868
T_* , K using (26)		456.9	481.7	516.2	528.3	539.9	558.8	608.1
$t_{i,s}$ using (26) for T_* according to (26)		76.514	9.124	0.659	0.153	0.1315	0.03993	0.00254
$t_{ig,s}$ using (30) for T_* according to (26)		83.221	9.896	0.714	0.165	0.142	0.04316	0.00275
$t_{ig,s}$ experimentally [6]		65	7.6	0.55	0.132	0.115	0.034	0.0022
T_{ig} , K using (28) for T_* according to (26)		466.9	492.8	529	551.3	553.9	573.9	625.9
Calculated values for T_* according to (26)	$t_{ig,s}$	103.95	8.980	0.654	0.151	0.1298	0.03932	0.0025
	Y_s	0.874	0.938	0.929	0.924	0.923	0.9184	0.906
Calculated values for T_* according to (28)	$t_{ig,s}$	129.385	9.86	0.715	0.165	0.1418	0.04296	0.00271
	Y_s	0.64	0.849	0.829	0.819	0.815	0.804	0.785
$T_{s,ig}$, K using (22) for $\varphi = 0,15$		446.7	470.4	503.2	523	525.7	543	590.2
Calculated values for $T_{s,ig}$ according to (22)	$t_{ig,s}$	82.73	8.02	0.586	0.1354	0.1164	0.03532	0.00225
	Y_s	0.965	0.978	0.975	0.974	0.973	0.971	0.967
$t_{i,s}$ using (29) for $T_{s,ig}$ according to (22)		67.348	8.03	0.584	0.1356	0.1168	0.03531	0.00226
$t_{ig,s}$ using (30) for $T_{s,ig}$ according to (22)		73.365	8.72	0.632	0.1467	0.1264	0.03818	0.00245
$t_{ig,s}$ using (27) for $T_{s,ig}$ according to (22)		220.186	27	1.932	0.4568	0.3792	0.1201	0.00734

Eqs.(1) and (4), describing the conservation of energy and the components of the solid propellant, are solved numerically and simultaneously in this work, by finite-difference method using the implicit scheme to ensure stability. The initial and boundary conditions are defined by eqs.(2), (3) and (5). Temperature and concentration were computed in 100 points, choosing the space grid step separately, for each value of external flux and heated propellant layer x_r , defined by eq.(19). The time increment was determined to satisfy the well-known stability condition $a\Delta t / \alpha_x \mathbf{f} < 1/2$.

The parameters characterizing the ignition process with different heat flux intensities of the double-base rocket propellant from [6] are presented in Table 1. The deviation between the ignition times numerically computed through correlated ignition temperature (by eq.(22)) and the experimental values ranges from 2 to 6% except for a very small value of heat flux ($\dot{q} = 0.01256$ MW/m² = 0.3 cal/cm²s) when it grows to 27%.

Reference [6] gives the times of ignition and solid double-based propellant surface flame setup measured experimentally, using ultrasonic sensors (Table 2).

Table 2

$\dot{q}_{ig} = 0.18428$ [MW/m ²]	$t_{ig} = 0.55$ s	$T_{ig} = 503$ K	$t_f = 0.63$ s	$p = 1$ bar
$\dot{q}_{ig} = 0.8918$ [MW/m ²]	$t_{ig} = 0.034$ s	$T_{ig} = 543$ K	$t_f = 0.04$ s	$p = 9$ bar

Higher values of heat flux decrease the ignition times and increase the difference between the flame setup and the ignition times ($t_f/t_{ig} = 1.145$ for the lower and $t_f/t_{ig} = 1.176$ for the higher flux level) and produces higher ignition temperatures.

Fig.1 illustrates the solid propellant temperatures during the ignition process in a layer near the surface (depth up to 1 mm) obtained numerically, by solving eqs.(1) and (4). The heat flux intensity of 0.041868 MW/m² (1 cal/cm²s) is very often used in experimental research. The figure clearly shows that the dominant reactions for the analysed model of this process occur on and immediately under the propellant surface. When the ignition temperature at the surface is achieved (470 K), the propellant temperature at a depth of $1 \cdot 10^{-3}$ m is approximately 340 K.

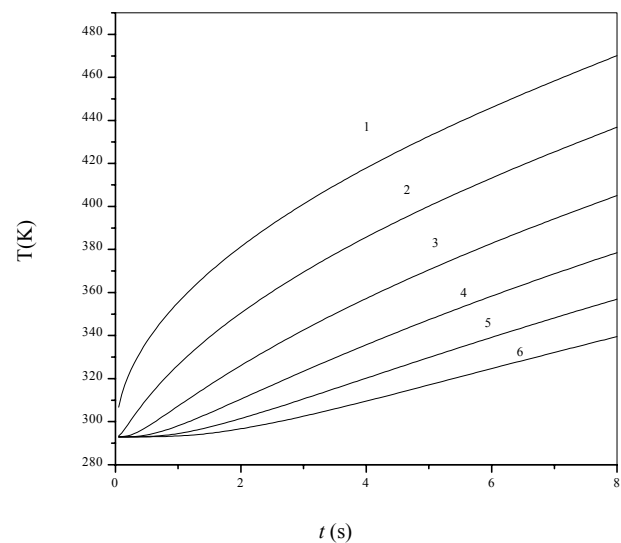


Figure 1. Time dependence diagram of the calculated temperatures in a layer near the surface of a double-base rocket propellant (thermophysical parameters from [6]) for igniting with a constant heat flux value $\dot{q} = 0.041868$ MW/m²: 1- T on the surface; 2- at $x = 2 \cdot 10^{-4}$ m depth; 3- $x = 4 \cdot 10^{-4}$ m; 4- $x = 6 \cdot 10^{-4}$ m, 5- $x = 8 \cdot 10^{-4}$ m; 6- $x = 1 \cdot 10^{-3}$ m

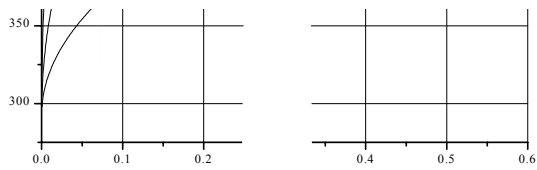
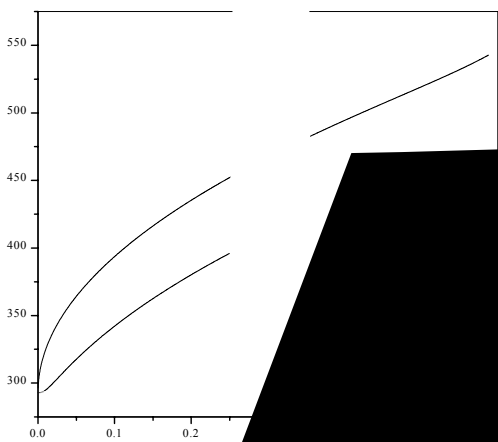


Figure 2. Diagram of the computed surface temperature buildup for double-base rocket propellant ignited by the following intensities of external heat flux: 1-0.18422 MW/m², 2-0.41868 MW/m² and 3-0.81736 MW/m².

face temperature buildup for double-base rocket propellant ignited by the following intensities of external heat flux: 1-0.18422 MW/m², 2-0.41868 MW/m² and 3-0.81736 MW/m².

The numerically obtained surface layer of the double-base rocket propellant „N” with an initial temperature of 300 K and a thermal conductivity of $\lambda = 0.1$ W/m·K added [7] for $\dot{q}_{ig} = 0.20934$ MW/m² is shown in Fig.3.

temperature distribution in the surface layer of the double-base rocket propellant „N” with an initial temperature of 300 K and a thermal conductivity of $\lambda = 0.1$ W/m·K added [7] for $\dot{q}_{ig} = 0.20934$ MW/m² is shown in Fig.3.



Primena toplotne teorije na analizu nekih slučajeva pripaljivanja čvrstih dvobaznih raketnih goriva

Analizirana je toplotna teorija pripaljivanja čvrstih raketnih goriva zasnovana na egzotermnoj hemijskoj reakciji u potpovršinskom sloju čvrste faze. Vremenski zavisne jednačine koje kontrolišu proces (održanje energije i komponenti) bile su rešene numerički radi dobijanja raspodele temperature i koncentracije u čvrstoj fazi. Izračunate vrednosti karakterističnih parametara su u zadovoljavajućoj saglasnosti sa većom grupom eksperimentalnih podataka iz literature. Tako, iako je uticaj reakcija u gasnoj fazi za vreme pripaljivanja dvobaznih raketnih goriva evidentan, pokazana je mogućnost korišćenja toplotne teorije pod određenim uslovima.

Cljučne reči: čvrsto raketno gorivo, dvobazno gorivo, pripaljivanje, sagorevanje.

Application de la théorie thermique à l'analyse de quelques cas d'allumage des propergols solides à double base

Le papier analyse la théorie thermique de l'allumage des propergols solides basée sur la réaction chimique et exothermique dans la couche sus-jacente de la phase solide. Les équations dépendantes de temps qui contrôlent le procès (conservation de l'énergie et des composantes) ont été résolues par la voie numérique afin d'obtenir la distribution de la température et de la concentration dans la phase solide. Les valeurs calculées des paramètres caractéristiques sont en concordance avec un large groupe des données expérimentales provenant de la littérature. Bien que l'effet des réactions dans la phase gazeuse pendant l'allumage des propergols à double base soit évident, on a démontré la possibilité d'utiliser la théorie thermique sous conditions particulières.

Mots-clés: propergol solide, propergol à double base, allumage, combustion.

