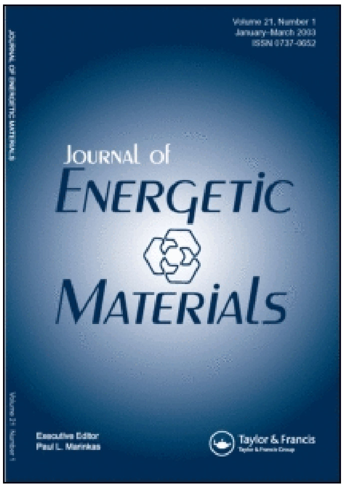

Journal of Energetic Materials
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713770432

Thermodynamic analysis of afterburning of detonation products in confined explosions

Waldemar A. Trzciński[a]; Józef Paszula[a]; Piotr Wolański[b]
[a] Military University of Technology, Warsaw, Poland [b] Warsaw University of Technology, Warsaw, Poland

To cite this Article Trzciński, Waldemar A. , Paszula, Józef and Wolański, Piotr(2002) 'Thermodynamic analysis of afterburning of detonation products in confined explosions', Journal of Energetic Materials, 20: 3, 195 — 222
To link to this Article: DOI: 10.1080/07370650208244821
URL: http://dx.doi.org/10.1080/07370650208244821

THERMODYNAMIC ANALYSIS OF AFTERBURNING OF DETONATION PRODUCTS IN CONFINED EXPLOSIONS

Waldemar A. Trzciński, Józef Paszula
Military University of Technology
Kaliskiego 2, 00 908 Warsaw, Poland

Piotr Wolański
Warsaw University of Technology
Nowowiejska 25, 00 665 Warsaw, Poland

ABSTRACT

In the paper, an attempt is undertaken to apply the thermodynamic theory of closed combustion, proposed by A. K. Oppenheim and co-workers, to analyse the process of afterburning of the detonation products of condensed explosives in a chamber filled with air. The principal assumptions of the theory are presented and the problem of combustion of fuel in a closed volume is formulated. The relations between thermodynamic parameters and fuel consumption are determined from the laws of conservation of volume, mass and energy. These relations are used to estimate the rate and heat effect of afterburning of the detonation products of some explosives in a steel chamber of 150 dm^3 volume. The influence of assumed degree of mixing of the combustion products and air on the mean pressure in the chamber is discussed.

Journal of Energetic Materials Vol. 20, 195-222 (2002)
Published in 2002 by Dowden, Brodman & Devine, Inc.

INTRODUCTION

Effects of turbulent combustion of the detonation products of condensed explosives have been studied recently in papers[1÷5]. Explosives of high deficit of oxygen were used in these investigations. The detonation products of such explosives are fuels themselves and, under some circumstances, they can react with oxygen from air, e.g., after detonation in closed volumes (vessels, chambers). In experimental investigations of afterburning of the detonation products, overpressure histories at the chamber wall are measured. To determine the effects of afterburning, charges of the explosive tested are detonated in the chamber filled with air or with inert gas. The averaged overpressure histories are the basis for estimation of the rate of combustion and the energy released. Moreover, from the averaged overpressures, TNT equivalents for the explosives tested can be determined for confined explosions[5]. The heat effect of afterburning of detonation products can be also measured in the calorimetric bomb[6-7] or estimated from the composition of products determined after detonation in the chamber[7÷9].

To estimate the rate of energy release in the chamber on the basis the measured pressure, the theoretical model was applied in papers[1-2,5], in which the non-equilibrium state of the reacting mixture was assumed. Apart from the pressure histories measured in the chamber filled with air and nitrogen, the results of thermochemical calculations were used in the procedure of determining the rate and final heat effect of combustion of the detonation products of TNT and its mixtures with RDX and Al.

In Ref.[3], the thermodynamic model was presented, in which a pressure in the reacting mixture was homogeneous but temperatures of the components, i.e., fuel (detonation products), oxidizer (air) and combustion products, were different. It was assumed that at the initial state all of the energy of detonation was stored in the motionless detonation products, which expanded to the average pressure measured in the chamber filled with inert gas. The model was applied for estimation of the rate and heat of afterburning of the detonation products of 875 g TNT in the chamber of 16.64 m^3 in volume.

The model[3] of the reacting mixture of fuel, oxidizer and combustion products was also applied in Ref.[4], in which the final heat of afterburning of the detonation products of TNT charges of small mass (about 1 g) in a 100 dm^3 vessel were determined. The initial state of air and detonation products was determined from the laws of conservation of volume and energy.

In this paper, the thermodynamic analysis of afterburning of detonation products in an enclosure is performed. In this goal, the model of three-component mixture (fuel, oxidizer, combustion products) and the theory of thermodynamics of closed combustion systems (Oppenheim and co-workers[10÷13]) are applied to estimate the rate and total heat effect of afterburning of the detonation products of chosen condensed explosives in a 150 dm^3 chamber. The main assumptions of the theory are presented and its use for analysing the process of afterburning is described. In particular, the influence of assumed degree of mixing of reacting mixture on the pressure is studied. Results of experiments performed for 25-g charges of TNT or TNT/RDX, with and without an aluminium additive, are used in the analysis. These results are signals of overpressure recorded after detonation of explosive charges in the chamber filled with nitrogen or air.

THERMODYNAMIC MODEL OF CLOSED COMBUSTION

Formulation of the Problem

Due to combustion of fuel in an enclosure, the pressure of closed gas increases. A part of the combustion heat is lost by reason of heat flow to the walls. However, if these losses are taken into account, there is an unambiguous relation between the fuel consumption and the pressure in an enclosure. Thus, the analysis of the combustion process and determination of combustion characteristics on the basis on the pressure history are possible.

Like as in Refs.[10÷13], let us consider a closed system, in which the exothermic processes take place as a result of transformation of reagents, R, into products, P. A rate of chemical reactions is so fast, that the transition from R to P, if they are mixed, is instant.

Fuel, Φ, and oxidizer, Ω, take part in reactions. In a closed combustion system they form non-stoichiometric mixture - charge, C. Therefore, the system, S, consisting of fuel, oxidizer and combustion products, is a multicomponent medium, in which the distribution of components in space is not taken into account.

However, the thermodynamic parameters of each component can be different. The internal energy and specific volume in the system are assumed to be additive.

It is assumed that the principal thermodynamic reference parameter is

$$w_k \equiv p_k \, v_k \ , \tag{1}$$

where p and v denote the thermodynamic pressure and specific volume, while $k = \Phi, \Omega,$ R, C, P and S.

The thermodynamic pressure is considered as spatially uniform. Hence, the effect of pressure gradient is disregarded, so that

$$p_k = p(t), \tag{2}$$

where t, the time, is the primary independent variable. In view of the fact, that p is a monotonic function of t and can be consider as a measure of time, all the thermodynamic variables are its functions only.

Under such circumstances, the balances of mass, volume and energy are expressed, respectively, as

$$m_\Omega + m_\Phi + m_P = m_S \tag{3}$$

$$v_\Omega \, m_\Omega + v_\Phi \, m_\Phi + v_P \, m_P = v_S \, m_S \tag{4}$$

$$u_\Omega \, m_\Omega + u_\Phi \, m_\Phi + u_P \, m_P = u_S \, m_S \tag{5}$$

where m_k is the mass, and u_k - the internal energy per unit mass. For closed volume, m_s and v_s are constant, but u_s may decrease due to heat losses. Since, the internal energy of the system can be expressed as $u_s = u_{si} - u_e$, where u_{si} denotes the internal energy at the initial state, i, and u_e - the heat losses per unit mass of the mixture.

After simple transformations, we obtain from Eqs. (3)÷(5):

$$Y_\Omega + Y_\Phi + Y_P = 1 \tag{6}$$

$$w_\Omega Y_\Omega + w_\Phi Y_\Phi + w_P Y_P = w_S \tag{7}$$

$$u_\Omega Y_\Omega + u_\Phi Y_\Phi + u_P Y_P = u_S \tag{8}$$

where Y_k is the mass fraction of the component k in the mixture.

The system of Eqs. (6)÷(8) is completed by the equation of state of components. Thermodynamic properties of the components are here presented on the so-called Le Chatelier diagram. This is a plot of the loci of states of reactants and products on the plane of specific internal energy, u, and thermodynamic reference co-ordinate, w, defined by Eq. (1)[12]. If components behave during the adiabatic processes as a perfect gas, the curves on the u - w plane are straight lines. An example of such a diagram is provided by Fig. 1 expressing the properties of a hydrogen/oxygen mixture ($2\ H_2 + 1.5\ O_2$). All the numerical results reported here are obtained by the use of the CHEETAH code[14]. Lines Ω and Φ are the loci of states of oxygen and hydrogen, respectively, compressed isentropically from the standard state (0.1 MPa and 293 K) to the pressure of 1.28 MPa, which is the final pressure of combustion of a stoichiometric mixture of hydrogen and oxygen in an adiabatic enclosure. Lines C, referring to the mixture of gases in the initial ratio, and R, corresponding to the stoichiometric mixture, are determined from the assumption of the additivity of specific volume and internal energy. The properties of the combustion products (water in gaseous state) are denoted by line P crossing points hp and uv. These points represent the states of equilibrium attained, respectively, at the initial enthalpy and pressure and at the initial internal energy and volume. Contrary to lines Ω and Φ, the entropy changes on line P. The curve of isentropic compression of gaseous water from ph point is shown on Fig. 1 by the dashed line. It is located very close to line P.

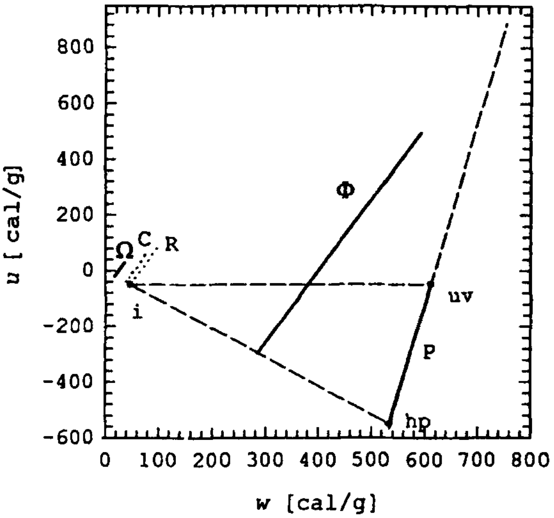

FIGURE 1: Le Chatelier diagram for $2\,H_2 + 1{,}5\,O_2$ mixture

Let us assume that the hypothetical process of combustion of fuel in a closed volume filled with oxidizer proceeds in the following way. At the initial state, i, a small amount of reagents maintained at constant pressure and enthalpy changes into products, i.e., the products reach the state hp. In the next step, the state of all the components changes immediately in the adiabatic way to fulfil the condition of constant volume of the mixture. The succeeding portion of reactants at line R (but from the point being different from point i) undergoes the transformation into the products at the state on line P, when pressure and enthalpy are at their values from line R. This process is repeated until the combustion process ends. Thus, the states of components in the adiabatic processes can change only alongside the lines $u_k = c_k w_k + q_k$ ($k = \Omega$, Φ, P). The method of solving the set of equations (6)÷(8) for the components, which the thermodynamic properties are expressed in terms of the Le Chatelier diagram, will be presented hereafter.

Solution of the Problem

The variable $Y \equiv Y_P$ is adopted as a progress parameter of the combustion process. The mass fractions of other components are expressed as functions of Y. At the initial state we have $Y = 0$, and from equation (6) the following relations can be obtained

$$Y_{\Phi i} = \frac{1}{1+\alpha} \tag{9}$$

$$Y_{\Omega i} = \frac{\alpha}{1+\alpha} \tag{10}$$

where $\alpha = Y_{\Omega i}/Y_{\Phi i}$ is the ratio of initial mass fractions of oxidizer and fuel in the mixture. The ratio of their mass contents in the stoichiometric mixture is denoted by σ. Henceforth, the mass fraction of oxygen is assumed to exceed that needed for full consuming of the fuel. From the equations (6), (9) and (10), the following expressions for Y_Φ and Y_Ω can be obtained

$$Y_\Phi = F_C - F_R\, Y \;, \tag{11}$$

$$Y_\Omega = 1 - F_C - \left(1 - F_R\right) Y \;, \tag{12}$$

where $F_C = \frac{1}{1+\alpha}$ and $F_R = \frac{1}{1+\sigma}$ are mass contents of the fuel in the initial mixture ($F_C = Y_{\Phi i}$) and in the stoichiometric one, respectively.

The final mass of products is

$$Y_f = \frac{F_C}{F_R} \; . \tag{13}$$

We normalise all the co-ordinates with respect to the initial state of oxidizer, i.e.,

$$W_k \equiv \frac{w_k}{w_{\Omega i}} \; , \tag{14}$$

$$U_k \equiv \frac{u_k - q_0}{w_{\Omega i}} \; , \tag{15}$$

$$P \equiv \frac{p}{p_i} \; , \tag{16}$$

where $q_0 = u_\Omega$ for $w_\Omega = 0$.

In normalised co-ordinates, the thermodynamic properties of the components on the Le Chatelier diagram are expressed by the lines

$$U_\Omega = C_\Omega W_\Omega \; , \tag{17}$$

$$U_k = C_k W_k - Q_k \qquad (k = \Phi, \mathrm{P}) \; , \tag{18}$$

and the thermodynamic reference parameters, except for the products, are related to pressure by polytropic functions

$$W_k = W_{ki} \, P^{1-\frac{1}{\gamma_k}} \qquad (k = \Omega, \Phi) \; , \tag{19}$$

where $\gamma_k = 1 + 1/C_k$.

From the volume balance (Eq.(7)), the parameter W_P can be expressed as a function of Y (for $Y > 0$)

$$W_P = W_R + \frac{W_S - W_\Omega - F_C\left(W_\Phi - W_\Omega\right)}{Y}, \tag{20}$$

where $W_R \equiv F_R W_\Phi + (1 - F_R) W_\Omega$.

Taking into account the linear relations (17)-(18), the balance equations can be solved for the products fraction

$$Y = \frac{\omega - 1 + k_P W_S + W_\Omega\left(1 - k_P\right) + F_C\left[k_\Phi\left(W_\Phi - W_{\Phi i}\right) + 1 - W_\Omega - k_P\left(W_\Phi - W_\Omega\right)\right]}{\Omega_P + W_\Omega\left(1 - k_P\right) + F_R\left[W_\Phi\left(k_\Phi - k_P\right) + W_\Omega\left(k_P - 1\right) - \Omega_\Phi\right]} \tag{21}$$

where $k_\Phi = C_\Phi/C_\Omega$, $k_P = C_P/C_\Omega$, $\Omega_P = Q_P/C_\Omega$, $\Omega_\Phi = Q_\Phi/C_\Omega$, $\omega = U_e/C_\Omega$.

The system is assumed to be isolated, i.e., $\omega = 0$. In this case, the relation is true: $W_S = W_{Si}\ P$, where $W_{Si} = F_C W_{\Phi i} + (1 - F_C)$.

From the equation (21) and relations (19), the mass fraction of the products, Y, as a function of the pressure P can be calculated. Due to the fact, that the pressure is unambiguous function of time, the equation (21) can be used to determine the rate of combustion on the basis of the measured pressure history.

APPLICATION OF THE MODEL

Experimental

The process of afterburning of the detonation products of condensed explosives was investigated in a chamber; it schematic diagram is shown in Fig. 2. The chamber was filled with nitrogen or air under a normal pressure. Charges of TNT, Tritonal (TNT/Al

85/15), Hexatol (TNT/RDX 50/50) and Hexatonal (TNT/RDX/Al 42.5/42.5/15) were detonated. Standard fuses were used to initiate the detonation of the 25-g mass charges. Signals of overpressure from two piezoelectric gauges located at opposite walls of the chamber were measured. To eliminate the influence of the gasdynamical processes on the averaged overpressure history, the gauges were placed in special cells (sockets) (Fig. 2). From 3 to 5 tests were made for each type of explosive and gaseous filler of the chamber. Selected overpressure records for TNT charges are presented in Fig. 3 by dotted lines. The time starts at the moment of the first reverberation of a shock wave at the chamber wall.

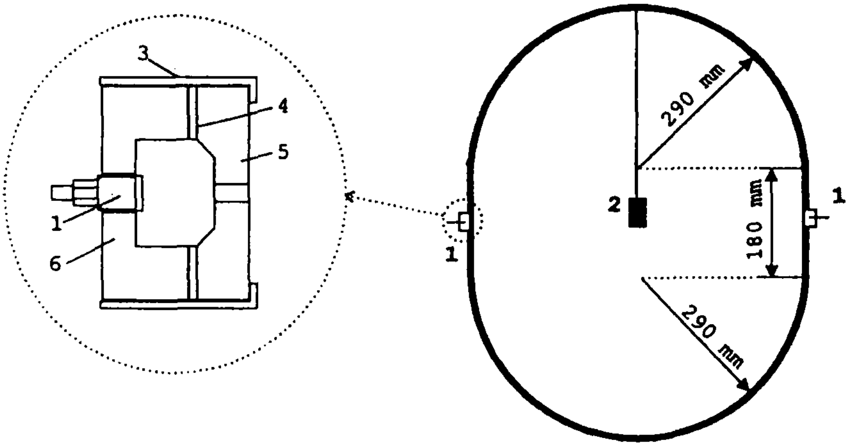

FIGURE 2: Schematic diagram of a chamber: 1 - pockets with pressure gauges, 2 - a charge of explosive, 3 - teflon cylinder sleeve, 4 - teflon separator, 5,6 - steel plates

The overpressure records have the oscillating nature. The main oscillations are caused by shock waves reverberation at the chamber walls. Their amplitudes decrease with time. There is observed "noise' on pressure histories of smaller amplitude and higher frequency. These disturbances are the result of turbulence of gaseous medium[3], reverberations of shock waves inside the sockets and vibration of the measuring system.

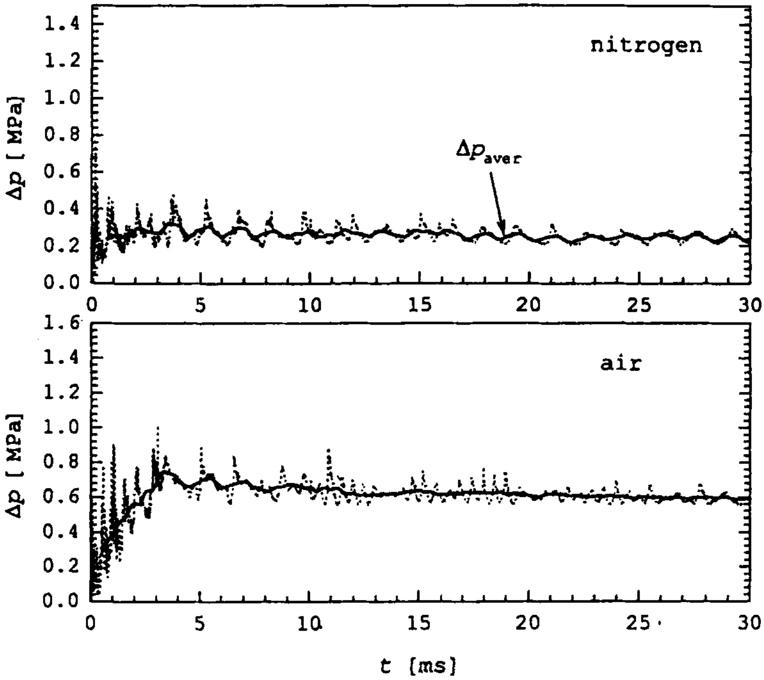

FIGURE 3: Variation of the overpressure (*dotted lines*) at the chamber wall after detonation of 25 g of TNT and averaged overpressure (*solid lines*)

The averaged overpressure histories were obtained by using the following formula:

$$\Delta p_{aver}(t) = \frac{1}{\tau} \int_{t-\frac{\tau}{2}}^{t+\frac{\tau}{2}} \Delta p\,(t')dt', \qquad (22)$$

where $\Delta p(t)$ is the measured overpressure, τ denotes a "window" in the averaging procedure. Chosen value of τ was about two times longer than the duration of the main peak on overpressure history. The results of averaging are presented in Fig. 3 by solid lines.

Taking into considerations the results obtained in all experiments performed for the given explosive and gaseous filler of the chamber, the mean overpressure history was determined. In the case of nitrogen in the chamber, it is assumed that the reduction of the mean overpressure is caused mainly by the heat flow to the chamber wall. Thus, the time-dependence of the mean overpressure can be approximated by the following function:

$$\Delta p_{apr}(t) = \Delta p_0 \, e^{-a(t-t_0)} \qquad (23)$$

where Δp_0 and a are constants, t_0 is the time corresponding to the first point on the averaged histories (t_0 = 0.75 ms). The parameter Δp_0 can be treated as the mean overpressure in the chamber with walls isolated adiabatically.

In the case of air filler, the combustion process influences the mean overpressure data. The averaged histories were approximated by the following function:

$$\Delta p_{apr}(t) = \left[\Delta p_0 + \left(\Delta p_m - \Delta p_0\right)\left(1 - b^{\frac{t-t_0}{t-t_k}}\right)\right] e^{-a(t-t_0)} \qquad (24)$$

where Δp_0 was determined for the given explosive in the chamber with nitrogen filler, Δp_m, b, and a are constants, t_k - the final time of observation of the combustion process (t_k = 30 ms). The calculated values Δp_0, a, Δp_m and b are presented in Table 1. Exemplary averaged histories of overpressure (pointed lines) and approximating curves (solid lines) are shown in Fig. 4.

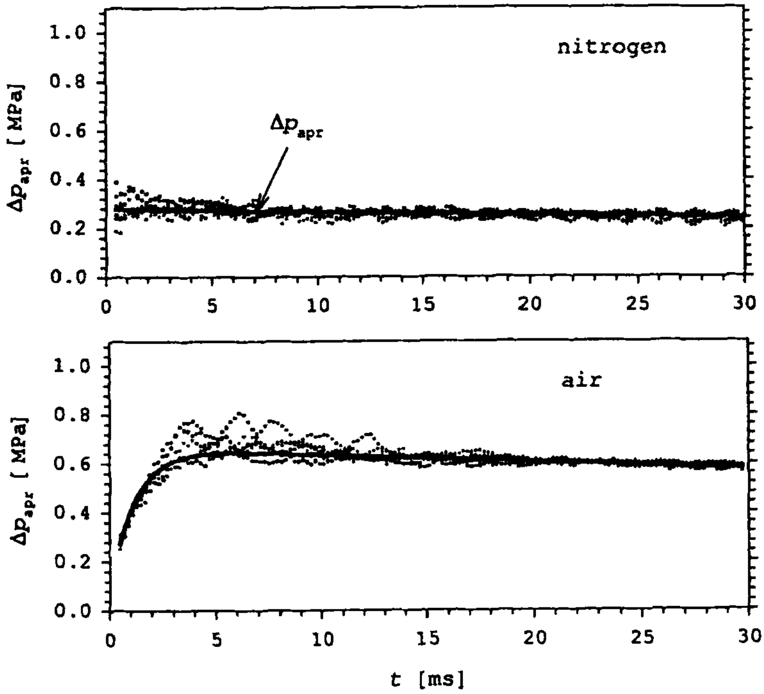

FIGURE 4: Summary of averaged overpressure for 25 g TNT and approximating lines

TABLE 1

Calculated parameters for the functions (23) and (24)

Explosive	Gas	Parameter of approximation			
		Δp_0 [MPa]	a	Δp_m [MPa]	b
TNT	nitrogen	0.278	0.0047	-	-
	air	0.278	0.0044	0.663	$5.712\ 10^{-6}$
Tritonal	nitrogen	0.288	0.0043	-	-
	air	0.288	0.0028	0.699	$8.903\ 10^{-6}$
Hexatol	nitrogen	0.294	0.0050	-	-
	air	0.294	0.0035	0.552	$5.542\ 10^{-10}$
Hexatonal	nitrogen	0.338	0.0036	-	-
	air	0.338	0.0042	0.635	$1.300\ 10^{-9}$

Determination of the Initial State

The energy released during the detonation of an explosive charge transfers into the kinetic and internal energy of air and kinetic energy of detonation products. In view of the fact that the A. K. Oppenheim theory[10÷12], in which the dynamic processes in a closed system are neglected, is to be used to described combustion of the detonation products, the detonation energy must be distributed between the internal energies of the detonation products and air. We assume that at the initial state the pressure in the chamber filled with air, p_i, is equal to the mean pressure determined experimentally for the nitrogen filler, i.e., $p_i = \Delta p_0 + p_0$, where p_0 is the atmospheric pressure. Thermodynamic properties of the detonation products of tested explosives and air under the initial pressure p_i are evaluated in the following manner. It is assumed that the detonation products expand along the Chapman-Jouguet (CJ) isentrope and reactions in the products are frozen at 1800 K[15]. Simultaneously, air is compressed adiabatically. We assume that the expansion process ends when pressure in the detonation products and air is just the same - p_r. The increase of the internal energy of air per gram of explosive is denoted by Δu_{ad}. The mechanical work done during adiabatic expansion of the detonation products from CJ-state to volume v_r, corresponding to the pressure p_r, is described by the relation[16]

$$W_r = -\frac{u_{CJ}^2}{2} + \int_{v_{CJ}}^{v_r} p\,dv \quad , \tag{25}$$

where u_{CJ} and v_{CJ} denote, respectively, mass velocity and specific volume evaluated at the CJ point.

In the next step, an isochoric process is assumed for the detonation products and air. Spatially uniform pressure increases to $p = p_i$. This process can be connected with transformation of the kinetic energy into the internal energy of gases. The increase of the internal energy of air and detonation products during the isochoric process is denoted by Δu_{is}. At the end of this process, the sum of energy of the detonation products and air differs from the expansion work given by Eq. (25). Thus, in final step, the states of the gases are assumed to change under constant pressure, p_i, to fulfil the balance of energy. In this process, the increase of enthalpy for the detonation products and air can be written in the following manner

$$\Delta h_\Phi = h_\Phi(v_{\Phi i}) - h_\Phi(v_{\Phi is}) \quad , \tag{26}$$

$$\Delta h_\Omega = h_\Omega(v_{\Omega i}) - h_\Omega(v_{\Omega is}), \tag{27}$$

where subscript "is" denotes the state of gases after the end of the isochoric process. The balance of energy in the chamber for the constant pressure changes can be written in the following way

$$m_{\Omega i}\,\Delta h_{\Omega} + m_{\Phi i}\,\Delta h_{\Phi} = m_{\Phi i}\left(W_r - \Delta u_{ad} - \Delta u_{is}\right) , \qquad (28)$$

where $m_{\Phi i}$ and $m_{\Omega i}$ are masses of an explosive charge and air, respectively. The volume of gaseous medium is restricted by the chamber volume, V_c. Thus

$$m_{\Omega i}\,v_{\Omega i} + m_{\Phi i}\,v_{\Phi i} = V_c \ . \qquad (29)$$

The set of equations (28)-(29) determines univocally the state of detonation products and air after ending all dynamic processes in the chamber. In this way, the initial conditions for fuel (detonation products) and oxidizer (air) are obtained.

The method described is applied to determining the initial states of gaseous mixtures for 25 g charges of the explosive tested. In the case of aluminized explosives, it is assumed that a part of aluminium does not react with oxygen during expansion of the detonation products in nitrogen. It was proved in Ref.[6] that in inert atmosphere about 70 and 80 % of aluminium reacted with the detonation products of Tritonal and Hexatonal, respectively. Calculated frozen compositions of the detonation products of explosives detonated in the chamber with nitrogen are presented in Table 2.

TABLE 2

Compositions of the detonation products of explosives tested

Detonation products [mol/kg]	Explosive			
	TNT	Tritonal	Hexatol	Hexatonal
N_2	6.562	5.625	9.835	8.405
H_2O	7.115	1.697	8.152	1.817
CO_2	4.933	0.937	4.931	0.883
CO	9.992	14.100	9.241	13.530
H_2	1.543	5.257	1.472	5.682
NH_3	0.0	0.005	0.007	0.006
CH_4	1.160	1.235	1.259	1.235
C_2H_4	0.006	0.0	0.0	0.0
CH_2O_2	0.004	0.0	0.0	0.0
C_s	1.397	9.392	6.394	2.795
Al	-	1.586	-	1.057
Al_2O_3	-	1.850	-	2.114

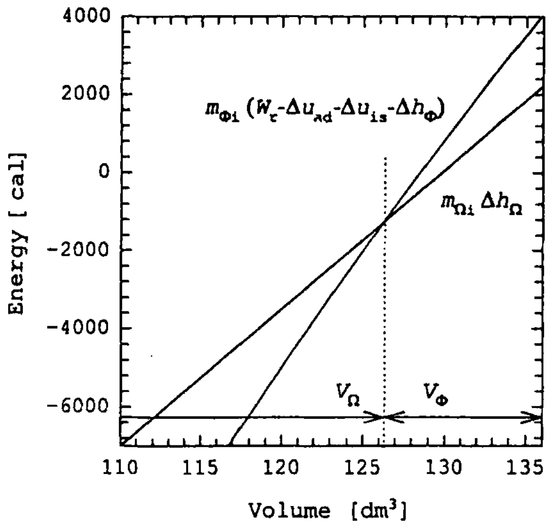

FIGURE 5: Diagram of energy balance in chamber at the initial state

To determine the thermodynamic state of the system of detonation products and air for the initial pressure p_i, equations (28)-(29) are solved graphically. Exemplary diagram of the energy balance is shown in Fig. 5. The calculated initial parameters of components of the mixtures tested are presented in Table 3. Beside of the specific volume, internal energy, enthalpy and polytropic exponent, the value of initial temperature is given for each component.

TABLE 3

Initial parameters of air and detonation products

Gas	Parameter	TNT	Tritonal	Hexatol	Hexatonal
Air	$v_{\Omega i}$ [cm^3/g]	699.1	645.4	625.5	654.3
	$h_{\Omega i}$ [cal/g]	154.9	144.0	140.9	178.9
	$u_{\Omega i}$ [cal/g]	92.2	84.1	81.8	110.1
	$T_{\Omega i}$ [K]	911	870	859	999
	$\gamma_{\Omega i}$	1.33	1.33	1.33	1.32
Detonation products	$v_{\Phi i}$ [cm^3/g]	912.4	1281.4	1418.1	1220.4
	$h_{\Phi i}$ [cal/g]	-808.5	-677.4	-614.7	-799.6
	$u_{\Phi i}$ [cal/g]	-891.4	-796.3	-748.6	-927.8
	$T_{\Phi i}$ [K]	1327	2322	1925	2024
	$\gamma_{\Phi i}$	1.18	1.16	1.20	1.18

Results of Calculations

Let us consider two models differing essentially in the degree of mixing of detonation products and air. In first model, we assume that the detonation products and air react in their stoichiometric ratio, and the combustion products and excess air are isolated adiabatically during the combustion process. The thermodynamic properties of the components of reacting mixture for all explosives tested are expressed in terms of the Le Chatelier diagrams. For example, the diagram in normalised co-ordinates is presented in Fig. 6 for the TNT charge. Points i denote the initial state, points f represent the final states corresponding to complete combustion of the detonation products.

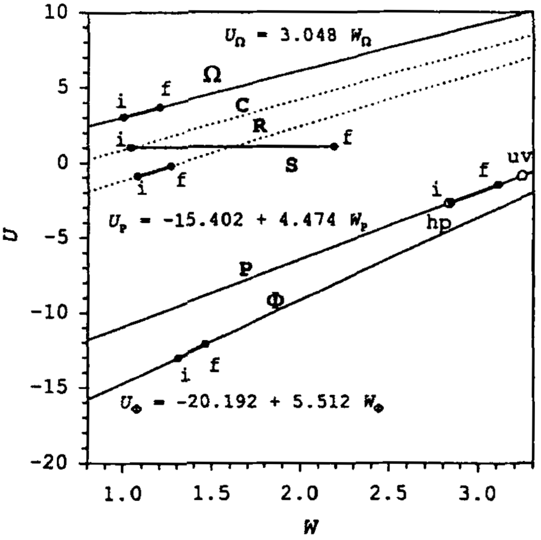

FIGURE 6: Le Chatelier diagram for confined combustion of 25-g TNT detonation products in air ($F_R > F_C$)

The values of coefficients $\mathcal{C}_k$ and C_k (k = Ω, Φ, P), obtained from the Le Chatelier diagram, are used to determine, from the Eqs. (19)÷(21), the dependence of the thermodynamic parameters W_k and the fraction of combustion products Y on the non-dimensional pressure P. If we assume, that the pressure in the chamber is equal at any time to the mean pressure obtained from the approximation of the experimental data, then the degree of fuel combustion, $x \equiv Y/Y_t$, can be determined as a function of time. Reduction of the mean pressure caused by the heat losses into the chamber walls is taken into account by the following manner

$$p(t) = p_0 + \left[\Delta p_{apr}(t)\right] e^{a(t-t_0)}. \qquad (30)$$

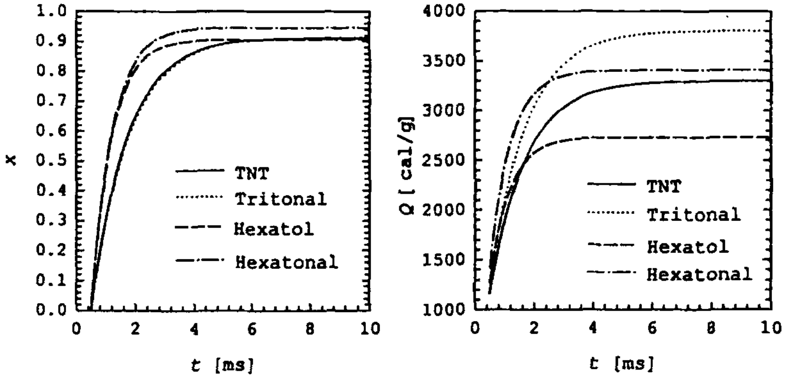

FIGURE 7: Burning rate and heat effect of combustion of the detonation products ($F_R > F_C$)

After calculation of the degree of combustion, we can determine the combustion heat released according to the relation $\Delta Q = x\ (Q_{com} - Q_{det})$, where Q_{com}, denotes the heat of combustion and Q_{det} is the heat of detonation of the explosive. The values of Q_{com} and Q_{det} are estimated on the basis of the calculated compositions of the products of combustion in oxygen atmosphere and detonation in an inert gas, respectively. The time-dependence of the combustion degree and the heat released in the chamber ($Q = Q_{det} + \Delta Q$) for the explosive tested is presented in Fig. 7.

The maximal degree of combustion of the dètonation products varies from 0.90 to 0.95 (Fig. 7). Meanwhile, the values of 0.68÷0.76 were obtained in Ref.[5] for the same charges. But in Ref.[5] the model was applied, in which the thermal equilibrium in the reacting mixture was assumed. In the model used here, two final components, i.e., air and combustion products, have different temperatures and physical properties. To investigate the influence of the degree of mixing of the components on the dependence of x on P, we have used the second model, in which it is assumed that air and detonation products react in the proportion of these gases in the chamber at the initial state. It means that reagents, R, are identical with the non-stoichiometric mixture, C, i.e., $F_R = F_C$. The Le Chatelier diagram for such a mixture is shown in Fig. 8 for TNT. The dependence of the degree of combustion and the heat released on the time is presented in Fig. 9 for the explosives tested.

From comparison of Figs. 7 and 9 it follows that, for the given explosive, the calculated degree of afterburning depends on the model assumed. The highest difference in the final degree of afterburning (about 30 %) is observed for Hexatonal. For all the explosives tested, the lower values of the degree are obtained for the model with more homogeneous distribution of the temperature in the reacting mixture. To explain this fact, the dependence of P on x calculated for both models is presented in Fig. 10 for TNT and Hexatonal.

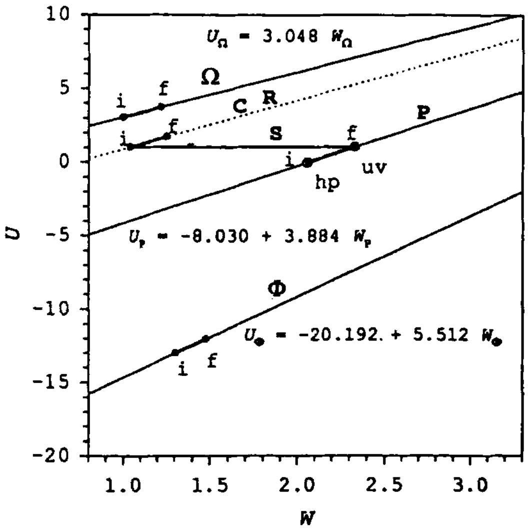

FIGURE 8: Le Chatelier diagram for confined combustion of 25-g TNT detonation products in air ($F_R = F_C$)

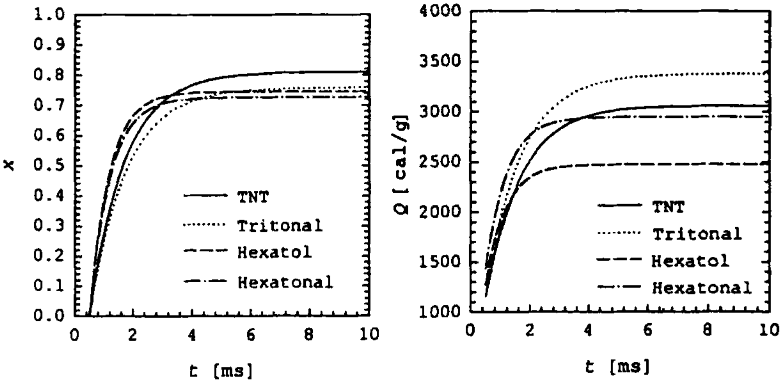

FIGURE 9: Burning rate and heat effect of combustion of the detonation products ($F_R = F_C$)

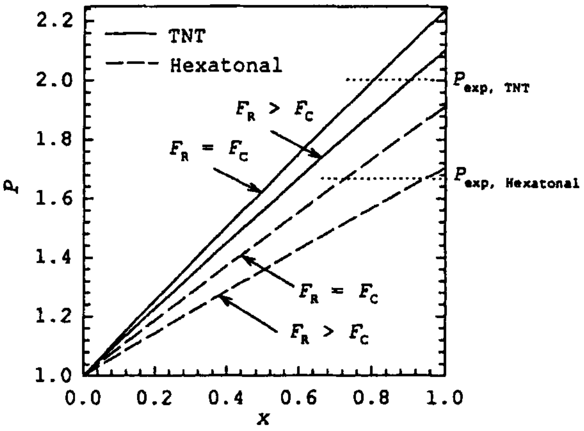

FIGURE 10: Dependence of the non-dimensional pressure on the degree of combustion of detonation products for the models used

From the Figure 10 it is visible that for the model with combustion products isolated adiabatically from air ($F_R > F_C$) the pressure in the chamber growths slowly with the degree of combustion than for the model, in which a part of air is mixed with the combustion products as an inert gas ($F_R = F_C$). It seems that such dependence is caused by the fact that the physical properties and contents of the combustion products are different for both the models. One of the physical parameters is a polytropic exponent. Its value influences the pressure of compressed gas. In Table 4, the values of this exponent for combustion products of explosive tested, and the final, maximal fractions of the products are given. For comparison, the exponent of air under conditions existing in the chamber is about 1.33, and that of the detonation products varies from 1.16 to 1.20 (see Table 3). Moreover, the initial states of the combustion products are different for both models (points i on lines P in Fig. 6 and 8).

TABLE 4

Parameters of combustion products for the models used

Explosive	$F_R > F_C$		$F_R = F_C$	
	γ_P	Y_f	γ_P	Y_f
TNT	1.22	0.516	1.26	1
Tritonal	1.20	0.527	1.23	1
Hexatol	1.22	0.379	1.27	1
Hexatonal	1.20	0.412	1.25	1

From the results presented in this work and in Ref.[5], the conclusion can be formulated that the degree of combustion estimated on the basis of the measured pressure history depends of the model assumed for describing the mixture of detonation products, air and combustion products. Generally, the degree of combustion is higher for the model, in which the state of the mixture is far from that being in the thermal equilibrium. To choose the model appropriate to the actual afterburning of detonation products in a closed volume, the final composition of the combustion products should be measured. The comparison of the degree of combustion determined from the products composition with that estimated from the pressure history enable us to verify the model. The chemical composition of the combustion products can be established by the use of the methods of gas chromatography[8-9].

SUMMARY

In the paper, the principal assumptions of the thermodynamic model of combustion in a closed volume are presented. The relationship between the mass fraction of fuel consumed by the exothermic process and the pressure in reacting system is given. The model is applied in analysing the process of afterburning of the detonation products of condensed explosives in an explosion chamber. The pressure histories measured in the chamber filled with nitrogen or air after detonation of charges of four high explosives are used. The initial state of fuel (detonation products) and oxidizer (air) in the chamber is determined. The thermodynamic properties of components of the reacting mixture are expressed in terms of the Le Chatelier diagram. From the solution of the inverse problem, i.e., estimation of the fraction of fuel consumed on the basis of the pressure, the time-dependence of the degree of combustion of the detonation products is determined.

Two models of combustion are considered. In the first model, fuel and oxidizer react in a stoichiometric proportion and the combustion products and excess air are isolated adiabatically each another during the combustion process. In the second model, the ratio of fuel to oxidizer in reactions is equal to their initial proportion in the closed volume. This means that the excess air is assumed to mix with the combustion products. The results obtained indicate that the time-history of consumption of the detonation product and the maximal heat effect estimated on the basis of the pressure measured in the chamber depend on the assumed means of

mixing of reacting gases. The estimated degree of combustion is higher in case of the model with gases being in thermal non-equilibrium.

REFERENCES

1. S. Cudziło, J. Paszula, R. Trębiński, W. A. Trzciński, P. Wolański, *Studies of afterburning of TNT detonation products in confined explosions,* Archivum Combustions, **17**, (1997), No.1-4.
2. J. Paszula, R. Trębiński, W. A. Trzciński, P. Wolański, *Afterburning of detonation products in an explosion chamber,* Proceedings of 29th International Annual Conference of ICT - Energetic Materials, Karlsruhe,1998.
3. A. L. Kuhl, J. Forbes, J. Chandler, A. K. Oppenheim, R. Spector, R. E. Ferguson, *Confined combustion of TNT explosion products in air,* Proceedings of the Colloquium on Gas, Vapor, Hybrid and Fuel-Air Explosions, Schaumburg, 1998.
4. P. Wolański, Z. Gut, W. Trzciński, L. Szymańczyk, J. Paszula, *Visualization of turbulent combustion of TNT detonation products in a steel vessel,* Shock Waves, **10**, (2000) 127-136.
5. W. A. Trzciński, J. Paszula, *Confined explosions of high explosives,* Journal of Technical Physics, **41**, (2000) 3.
6. W. A. Trzciński, J. Paszula, S. Cudziło, *Experimental and theoretical estimation of the heat of afterburning of detonation products in a calorimetric bomb* (in Polish), Biul. WAT, **49**, (2000) 12.

7. D. L. Ornellas, *Calorimetric determinations of the heat and products of detonation for explosives: October 1961 to April 1982,* Report UCRL - 52821, Lawrence Livermore National Laboratory.

8. F. Volk, F. Schedlbauer, *Energy output of insensitive high explosive by measuring the detonation products,* Propellants, Explosives, Pyrotechnics, 18, (1996) 332-336.

9. F. Volk, F. Schedlbauer, *Analysis of post detonation products of different explosive charges,* Propellants, Explosives, Pyrotechnics, 24, (1999) 182-188.

10. A. K. Oppenheim, *Dynamic features of combustion,* Phil. Trans. R. Soc., London, AA 315, (1985) 471-508.

11. A. K. Oppenheim, *Quest for controlled combustion engines,* SAE Transactions, The Journal of Engines, 97, (1988) 6.

12. A. K. Oppenheim, J. A. Maxson, *Thermodynamics of combustion in an enclosure,* Progress in Astronautics and Aeronautics, New York, (1991) 365-382.

13. A. K. Oppenheim, J. E. Barton, A. L. Kuhl, W. P. Johnson, *Refinement of heat release analysis,* SAE Paper, 970538, 1997.

14. L. E. Fried: *CHEETAH 1.39 Users Manual,* UCRL-MA-11754 Rev. 3, Lawrence Livermore National Laboratory, Livermore, CA, 1996.

15. P. C. Souers, J. W. Kury, *Comparison of cylinder data and code calculations for homogeneous explosives,* Propellants, Explosives, Pyrotechnics, 18, (1993) 175-183.

16. W. Ficket, W. C. Davies, *Detonation,* University of California Press, Berkeley, 1979.